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OPACITY OF HIGH-TEMPERATURE AIR

by

B. H. Armstrong,

R. R. Johnston and P. S. Kelly

Lockheed Missiles & Space Company

Contract AF 29(601)-5006

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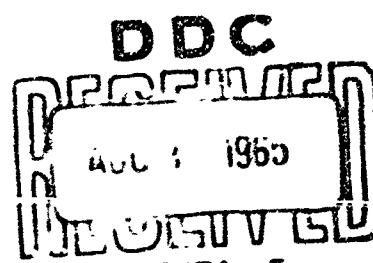
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FOREWORD

The opacity calculation described in this report was performed by B. H. Armstrong, R. R. Johnston, P. S. Kelly, O. R. Platas, and D. J. Colvin of the Lockheed Missile and Space Company, Sunnyvale, California under Contract AF 29(601)-5006. The research was funded under DASA Project 5710, Subtask 07.003, Program Element Number 7.60 06.01 5

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Inclusive dates of research were 15 January 1962 to 15 November 1964. The report was submitted in June 1965 by Lt R. Harris, WLRT, the Project Officer.

This report has been reviewed and is approved.

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ABSTRACT

A new calculation of the opacity of high-temperature air ($kT = 1 - 20 \text{ eV}$) is carried out. Line (bound-bound) transitions are included and LS term splitting of configurations is accounted for in the $n = 2$ and 3 levels. The primary purpose of the calculation is to remove the hydrogenic approximation to the dominant photoelectric and line transitions. In place of the hydrogenic approximation, Hartree-Fock-Slater matrix elements are used for the line transitions. For the photoelectric transitions, a combination of the Burgess-Seaton extension of the Coulomb approximation, and a high-energy acceleration-matrix-element Born approximation is employed. Comparisons are carried out with experiment and with previous calculations. A review and discussion is presented of the statistical mechanics of ionized gases, and some new results pertinent to the calculation of occupation numbers are presented.

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Section I INTRODUCTION

The transport of electromagnetic energy through the atmosphere is governed by the equation of radiative transfer (Refs. 1, 2, and 3)

$$-\frac{1}{\mu_\nu} \frac{dI_\nu}{ds} = I_\nu - J_\nu \quad (1.1)$$

where I_ν is the specific intensity of the radiation, ds the element of length, and J_ν the source function. This equation is in general very difficult to solve, and an extensive literature has accrued, principally in the field of astrophysics, dealing with its solution for various model problems and in various degrees of approximation. The principal physical parameter that enters any solution of this equation is the absorption coefficient μ_ν , and it is this absorption coefficient for air and its constituents that constitutes the subject of the present report. We will restrict ourselves to atomic absorptions by elementary interactions; molecular absorption and absorption arising from collective modes of excitation involving long-range forces will not be considered. The calculations discussed in this report are an outgrowth of work carried out at Lockheed Missiles & Space Company and at General Atomic over a period of six or seven years. The reports (Refs. 4 through 8) issued by both organizations during this period, as well as the comprehensive report due to Harris Mayer (Ref. 9) provide an adequate introduction to the problem. Therefore, we will not give a detailed discussion of the basic theory but only the background and definitions needed for an understanding of the calculations reported here.

Our principal aim has been to remove most of the hydrogenic approximations made in the past work by use of more realistic matrix elements, and by use of as much detail as possible in the description of photoelectric edges and spectral lines. We have used

the best theoretical predictions available for the rather massive numbers of atomic transitions considered and have tried to avoid unjustified physical assumptions as far as possible. Our formulation draws heavily on the work performed by our colleagues at General Atomic. We have attempted to combine their previous experience with ours to obtain what we hope are the best results for air absorption coefficients to date.

The absorption coefficient μ_ν can be written as

$$\mu_\nu = \sum_{S, i, j} N_{S_i} \sigma_{Sij}(\nu) \quad (1.2)$$

in terms of the occupation numbers N_{S_i} (particles cm^{-3}) for the state i of the species S , and the cross sections $\sigma_{Sij}(\nu)$ for a transition from state i to j of the species S . We have employed occupation numbers resulting from previous calculations (Refs. 6 and 10) which cover a temperature range from ~ 1 to 20 eV and a density range from \sim normal density to $\sim 10^{-5}$ normal density. The atomic transitions for which cross sections have been computed are the photoelectric (bound-free) and line (bound-bound) transitions. The free-free and Compton scattering contributions included in our mean absorption coefficients were obtained from our previous calculations (Refs. 4 and 5).

If one assumes that conditions of local thermodynamic equilibrium prevail, the source function in the transfer equation (Eq. 1.1) becomes the well-known Planck function

$$B_\nu(T) = \left(\frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/kT} - 1} \right)$$

plus a term that accounts for induced emission. There are then two limiting cases for which simple solutions to the transfer equation exist. If the optical depth $\mu_\nu x$ of the

radiating sample of gas is small* ($\mu_\nu x \ll 1$), where x is the sample dimension in the direction of radiation, the radiant energy emitted by the sample is given in terms of the Planck mean absorption coefficient:

$$\bar{\mu}_P = \frac{\int \mu'_\nu B_\nu(T) d\nu}{\int B_\nu(T) d\nu} \quad (1.3)$$

where $\mu'_\nu = [1 - \exp(-h\nu/kT)]\mu_\nu$. If the optical depth is large ($\mu_\nu x \gg 1$), one passes to the diffusion limit, and the emission of radiant energy is governed by the Rosseland mean absorption coefficient:

$$\frac{1}{\bar{\mu}_R} = \frac{\int \frac{1}{\mu'_\nu} \frac{\partial B_\nu(T)}{\partial T} d\nu}{\int \frac{\partial B_\nu(T)}{\partial T} d\nu} \quad (1.4)$$

Based on the relevant atomic theory (which will be described in succeeding chapters) an IBM 7094 computer called PIC has been devised to compute the photoionization cross sections and absorption coefficients. Another program, MULTIPLET, has been constructed to compute the atomic-line contribution. The input information consists of a list of the possible atomic states present in the gas and, for each of these, its spectroscopic description, energy, and occupation number. From this input each program computes and constructs an atlas of the parameters needed to adequately define the absorption coefficient.

The need for the atlas in the case of lines arises from the difficulties that would be associated with attempting to store or print the detailed shapes of the very narrow lines that appear at low, and even moderate, densities. The frequency interval

*For very strong spectral lines this may not be a physically realizable situation. See Ref. 8 for a discussion of this point.

required for this task would be so small that the tabular output would be prohibitively massive. Instead of attempting to tabulate this quantity of numerical absorption coefficient values, the wings of the narrow lines and the entire profiles of broad lines are printed as an additional pseudo-continuum. The parameters that describe the central portions of the narrow lines may then be obtained from the atlas. They can be used at the time of the computation by any subroutine one wishes to insert which compresses, arbitrarily integrates, or averages out part of the frequency dependence. The two such subroutines that we have employed are those which compute the Planck and Rosseland mean absorption coefficients. An atlas has also been devised for the photoelectric transitions. Although it is not needed in this case to compress the frequency dependence, it is still convenient since much edge-splitting detail is accounted for.

The atlas defining each of the individual atomic processes may also facilitate interpolation to gas temperatures and densities intermediate to those we have used.

By using the MULTIPLET line code in conjunction with the PIC code, total frequency-dependent or mean absorption coefficients have been computed. The results of this combined photoionization and line opacity program (PHLOP) for the mean absorption coefficients are presented in Sec. VI. Before proceeding to these results, we now embark on a detailed description of the various sub-computations involved. In Sec. II, a discussion is presented of our atomic state descriptions and lumping conventions. Section III gives a brief description of our previous occupation-number theory and the fundamental research which we have undertaken toward the ultimate aim of improving these numbers. The line transition theory is presented in Sec. IV, and the photoionization theory in Sec. V. The final results for the mean opacities obtained are in Sec. VI. In the appendices are provided information pertaining to the computer programs we have developed and listings thereof, and a more detailed description of our statistical mechanics research.

Section II ATOMIC-STATE CONVENTIONS

At a given temperature and density the state of the gas as a whole – assumed to be in thermodynamic equilibrium – is defined by the most probable number of atoms in each state of excitation of every charge state of every species present. The probability of occupation of an atomic state, the occupation number, is obtained from a statistical mechanical calculation of the classical grand canonical partition function (Sec. III), utilizing the energies of every atomic state assumed to be occupied. Thus the initial information necessary is the set of all atomic states under consideration and the energies of each relative to the ground state of the neutral atom of the species.

With each charge state (or state of ionization) there are associated a great many states of the remaining electrons. Some of these have been observed experimentally and are conveniently tabulated by Moore (Ref. 11). However, the majority of states, especially for the highly ionized atoms, have not been observed, and their energies must be estimated.

A particular atomic state is characterized by a core configuration – identified by the label γ – and an external electron with principal quantum number n and angular momentum quantum number l . The cores which have been considered consist of a closed K-shell with the 2s and 2p electrons coupled in all possible ways. A complete list of the atomic cores and their labels γ is found in Table II-1.

For each core state the outer electrons (n, l) will be in one of a large number of possible states, each coupling in a variety of ways to the core and leading to the usual multiplet structure. Russell-Saunders L-S coupling is assumed throughout

and total-angular-momentum splitting is consistently ignored. Occupation numbers have been evaluated for states with n -values up to 30, but the present calculation restricts n to be less than 17, as line merging (Sec. IV) tends to smear states with higher principal quantum number into the continuum. When the external electron state is equivalent to one of those in the core, the resulting state cannot be considered as belonging to any one core. For convenience such states are assigned to the core with the lowest excitation for the appropriate configuration.

States with only partially filled K-shells have not been included, as the energies of such states is sufficiently large to ensure negligible occupation at the temperatures being here considered. Similarly excluded are multiply excited states containing more than one electron with principal quantum number greater than two. For such states the energies and the theoretical techniques for their treatment are poorly known. As initial states their energies are so large as to result in small occupation. However, the neglect of such states as final states in bound-bound transitions rules out consideration of the phenomenon of auto-ionization which may make a measurable contribution to the photoionization cross section (Ref. 12). Further, atomic sum rules will not be strictly satisfied.

When known, the experimental energy values are used. Estimates of the energies of the remaining states were made by the Bacher-Goudsmit method, extrapolation of isoelectronic sequences, or constant quantum defect methods as described in Ref. 4.

As the occupation-number calculation depends only on the energy of an atomic state, it is convenient to combine states of nearly equal energy and to exploit the well-known sum rules over Wigner coefficients in the evaluation of the optical transition probabilities. The following conventions have been adopted for this combining or summing of states:

- (I) $n = 3$ Summed over total angular momentum L for given multiplicity $(2S + 1)$ when experimentally the L -splitting of the levels is much less than the S -splitting or when the energies are poorly known (Labelled: $L = 9$)

(ii) $n \geq 4$ Summed over all L-S terms (Labelled: $2S + 1 = 0$, $L = 0$)

(iii) $6 \leq n < 9$ Summed over electron angular momentum $l \geq 4$
(Labelled: $l = 4$)

(iv) $n > 9$ Summed over all values of the electron angular momentum (Labelled: $l = 0$)

Each atomic state is specified by an identification number ($i\gamma n l S L$) and the energy of the state (in eV relative to the ground state of the neutral atom of the species):

- i is a two-digit designation of the species and charge state: 01, 02, etc. for oxygen I, oxygen II, etc; and 11, 12, etc, for nitrogen I, nitrogen II, etc.
- γ is the two-digit designation of the core, as listed in Table II-1.
- n (two digits) is the principal quantum number of the excited electron or outermost populated shell
- l is the orbital angular momentum of the excited electron or outermost populated shell (summation conventions iii and iv)
- $(2S + 1)$ is the spin multiplicity (summation convention ii)
- L is the total orbital angular momentum (summation convention i and ii)

Table II-1
ATOMIC CORE CONFIGURATIONS

O-I	$1s^2 2s^2 2p^3 (4S) n l (2S+1 L)$	$\gamma = 1$
	(^2D)	2
	(^2P)	3
	$2s 2p^4 (4P)$	4
	(^2D)	5
	(^2S)	6
	(^2P)	7
	$2p^5 (2P)$	8

Table II-1 (cont'd)

O-II, N-I	$1s^2$	$2s^2$	$2p^2$	$(^3P)_{n\ell} (^{2S+1}L)$	$\gamma = 1$
				(^1D)	2
				(^1S)	3
	$2s$	$2p^3$	(^5S)		4
				(^3D)	5
				(^3P)	6
				(^1D)	7
				(^3S)	8
				(^1P)	9
		$2p^4$	(^3P)		10
				(^1D)	11
				(^1S)	12
O-III, N-II	$1s^2$	$2s^2$	$2p$	$(^2P)_{n\ell} (^{2S+1}L)$	$\gamma = 1$
			$2s$	$2p^2$	(^4P)
					(^2D)
					(^2S)
					(^2P)
		$2p^3$	(^4S)		6
				(^2D)	7
				(^2P)	8
O-IV, N-III	$1s^2$	$2s^2$		$(^1S)_{n\ell} (^{2S+1}L)$	$\gamma = 1$
		$2s$	$2p$	(^3P)	2
				(^1P)	3
		$2p^2$	(^3P)		4
				(^1D)	5
				(^1S)	6
O-V, N-IV	$1s^2$	$2s$		$(^2S)_{n\ell} (^{2S+1}L)$	$\gamma = 1$
			$2p$	(^2P)	2
O-VI, N-V	$1s^2$			$(^1S)_{n\ell} (^{2S+1}L)$	$\gamma = 1$

Section III

STATISTICAL MECHANICAL THEORY OF OCCUPATION NUMBERS*

BACKGROUND

A basic assumption in this work is that the absorption coefficient for radiation at frequency ν may be expressed as a sum of terms, each of which represents the absorption of radiation by particles in state i , and can be written as a product of two factors the cross section for a transition from i to an appropriate final state j , and the number of particles in state i . This assumption may be somewhat inaccurate at higher densities because transitions to j may be suppressed by "exclusion principle" effects if most of the j states are already occupied and because collective "plasma oscillations," which cannot be represented correctly in terms of individual atomic energy levels, may be involved in the absorption of radiation. It is assumed that such effects are unimportant. Thus, in the notation used in this report,

$$\mu(\nu) = \sum_{i,j} N_{i\nu} \sigma_{ij}$$

The procedure used to calculate the cross sections σ_{ij} is described in other sections; here we shall summarize the methods used to find the occupation numbers $N_{i\nu}$.

In general the calculation of occupation numbers for a partially ionized gas with arbitrary conditions of temperature, pressure, density, composition, radiation flow, and other factors (all of which may vary from one place to another) is a very difficult problem that is regarded as being for the most part beyond the reach of present-day theoretical physics. It is probably not unfair to say that the large amount of research devoted to this subject in the past few decades has succeeded only in developing some

*This section was written by LMSC consultant, Stephen Brush.

simple approximate methods that may be of limited validity when the physical conditions are of certain especially simple types; but that even then a direct experimental check of the theory is not usually possible. This situation is expected to improve in the next few years, however, as various laboratories develop facilities for studying high-temperature plasmas. In the meantime there is an urgent need for further theoretical work; indeed, even the interpretation of experimental results (such as the determination of the temperature of a plasma) depends heavily on theoretical ideas.

For theoretical discussions it is convenient to distinguish between two basic types of physical systems: equilibrium and nonequilibrium. (A third category, the non-equilibrium steady state, is also useful in some cases but will not be needed here.) The nonequilibrium case is the most general, since it includes in principle an infinite number of values for a large number of physical variables, whereas the equilibrium case requires that most of these variables have the value zero. The variables we have in mind here are those that describe the change of properties from one place to another in space, or the change of properties with time. Thus an equilibrium system can be characterized by a constant density, temperature, pressure, and composition, whereas the description of a nonequilibrium system involves the space- and time-derivatives of these quantities as well.

Despite the apparent artificiality of the equilibrium system in the context of most realistic problems involving radiation flow, it has two distinct advantages: (1) there exists a well-established and fairly simple theoretical technique for computing its properties; (2) it represents the best possible guess (in the sense of statistical estimation theory) as to the state of a physical system if only the temperature and density are known and definite information about other physical variables is lacking; and, moreover, it represents the final state which any system will eventually reach if left to itself without external disturbance.

To illustrate the difference between equilibrium and nonequilibrium theory, consider the case of absorption of radiation by air, with which this report is concerned. First

of all, we need to specify the initial state of the system before it receives any radiation. In equilibrium theory we can do this (at least approximately) as soon as we know the temperature and density, by assuming that the probability of each possible state is given by the Maxwell-Boltzmann distribution law. Calculational difficulties arise when we attempt to find the energy of each state, but as long as the density is not too high we can use tabulated spectroscopic data for the various individual atomic species, making small corrections for the effects of interactions of different atoms with each other. The important point is that only one piece of information is needed for each state: its energy. In the nonequilibrium theory there is no definite prescription for specifying the initial state, unless the temperature is so low that one can assume that there are no free electrons or ionized atoms, and that all the atoms are in their lowest electronic state. The temperature is not that low for the actual situations of interest in this report, so there is no such easy way out; and, unless we happen to have previously solved a problem involving the calculation of occupation numbers in radiation-flow situations, we would probably end up by assuming an equilibrium distribution for the initial state.

Now imagine that the radiation flow is "turned on" and a small number of photons of specified frequencies are absorbed, causing transitions from certain initial states to other states. The system will now have a different set of occupation numbers because of these transitions. In order to compute this new state we need to know all the cross sections for transitions between states. Presumably we already know the cross sections for transitions induced by photon absorption, since these are involved in the other part of the problem anyway; but in addition we will need to know all the cross sections for spontaneous radiative transitions, ionization by free electrons, collision cross sections, etc., since all kinds of complicated physical processes are going on in the gas at the same time as it is absorbing radiation. To treat the problem from the exact non-equilibrium viewpoint, consequently, would require a huge amount of input information about the physical properties of all the atomic species, as well as an enormous amount of computation in order to follow the time-evolution of the system through various sets of occupation numbers. In addition, the computation might have to take account of spatial variations.

At this point, to get any answer at all, one usually makes the additional assumption that the process is "linear" - one ignores the compounded effects of radiation changing occupation numbers which in turn would change the absorption of the next batch of radiation, and simply calculates the rate of absorption for very small amounts of radiation. The absorption coefficient is in fact defined as the ratio of the amount absorbed to the amount received, in the limit as both these quantities go to zero. To use such an absorption coefficient in problems involving a finite amount of radiation, one must assume that the internal relaxation processes in the gas will drive it back to equilibrium faster than the absorbed radiation can push it away from equilibrium. The calculation of occupation numbers need then be done only once for each specified density and temperature, and does not have to be repeated in order to take account of the effect of the radiation already absorbed.

As soon as we agree to restrict ourselves to equilibrium occupation numbers, we can effect a great simplification in the problem; we need only calculate the probability of each possible state of the system, without worrying about how one state follows another in the course of time. No information about cross sections for transitions between states is needed, but only the energies of the individual states. (It might be objected that we cannot calculate the energies unless we know the forces between the particles, and if we knew the forces then we could also calculate the cross sections. This is true in principle, but there is still an immense difference in practice between equilibrium and nonequilibrium calculations.)

In the following subsection we shall outline briefly the standard theory of statistical equilibrium in ionized gases. In a subsequent subsection, we shall discuss the method actually used to compute the occupation numbers used in our computer code for absorption coefficients. Finally, we shall summarize recent theoretical work performed under the contract to improve the method. The details of this work are presented in Appendix A. (Sects. A.1 and A.2); Sect. A.3 contains a derivation of formulas for average potentials and potential fluctuations in a plasma. This is of considerable value in actual applications of the theory presented in Sect. A.1.

STATISTICAL EQUILIBRIUM IN IONIZED GASES

To illustrate the principles of the theory, we consider first the following simplified model for an ionized gas. We have N atoms, each consisting of a nucleus of charge Z , mass M , and any number of electrons from 0 to Z . In addition there are N_e free electrons, where N_e is such that the system as a whole is electrically neutral. Each atom has a set of energy levels E_0, E_1, \dots ; in general, the nature of the levels would depend on the number of electrons in the atom, and, to a lesser extent, on the number of free electrons and other atoms and ions in the gas. However, we shall ignore such effects for the moment. Each energy level is characterized by a degeneracy factor g , which represents the number of levels having the same energy; as far as the statistical mechanical theory is concerned, we can group such levels together, although in the calculation of cross sections they must be treated separately.

We wish to know the average number of atoms of various degrees of ionization: $N_0 \dots N_Z$ for atoms with 0 to Z electrons removed from the neutral atom; and also the number of ions by which each of the various energy levels is occupied. The most direct way to solve the problem is to calculate first the distribution of kinetic energy among the atoms (even though we are not interested primarily in the kinetic energy) and then deduce from this the distribution over the various energy levels. In the usual terminology, we first derive the Maxwell distribution of velocities, and then generalize this to the Boltzmann distribution of energies. We refer to the standard texts on statistical mechanics for the details of the derivation and merely summarize it here. We shall also need the Gibbs grand canonical ensemble which gives the distribution of particles of different kinds in a mixture, in the case when the number of particles is not kept fixed.

We first make the postulate of equal a priori probability of all microscopic states of the system. This means, for example, that if the system as a whole has a fixed total kinetic energy K , then all possible ways of dividing this energy among the atoms are equally probable. The justification for this postulate is that we have no reason for assuming that any one way of distributing the energy is more probable than any other.

This postulate is rather awkward to apply as it stands, for it implies that the kinetic energy of any one atom cannot be found until we know the energies of all the others. In fact, however, it seems reasonable that if the number of atoms is very large, the energy of an individual atom will depend only on the average temperature of the system, as determined by its surroundings, and not on the precise values of the energies of the other atoms in the system. To make use of this idea of average temperature, we imagine that our system of N atoms is only a small part of a much larger system of N' atoms; it can exchange energy with the other atoms so that its own total energy is no longer strictly constant but will fluctuate around an average value. This hypothetical construction is known as the canonical ensemble in statistical mechanics: in a certain sense it is more realistic than the original model with fixed total energy, since we do not usually know the precise value of the energy of an isolated system, but rather the temperature of a system interacting with its surroundings.

We need one further assumption in order to apply the postulate of equal a priori probability of microscopic states: we need to know what those states actually are. If we knew, for example, that each atom could have only certain values of kinetic energy, namely integer multiples of some basic energy-unit E_0 - $\{k = 0, E_0, 2E_0, \dots, E_1\}$ - where E_1 is the fixed total energy of all N' atoms, then the problem would be well-defined. For any given energy of the first atom, k_1 , the second could have energies from 0 to $E_1 - k_1$, the third could have energies from 0 to $E_1 - k_1 - k_2$, and so forth; the energy of the last atom would be completely determined by the others. By combinatorial analysis we could determine how many arrangements correspond to giving energy k_j to the j^{th} atom, and then take the limit as E_1 goes to zero while N' goes to infinity but always remains proportional to N' .* The result is that the

*Although this derivation was first published by Boltzmann nearly a century ago, it is not available in most modern textbooks, so we shall outline it briefly. Suppose that the total energy E_1 of N' atoms has been divided into p units of magnitude E_0 . If $N' = 3$, we can choose k_1 and k_2 , and k_3 must be equal to $E_1 - k_1 - k_2$. If $k_1 = E_1$ there is only one microstate since k_2 and k_3 must both be zero. If $k_1 = (p - j)E_0/p$, then k_2 can have $j + 1$ possible values, from 0 to $(j/p)E_1$. The total number of microstates is therefore

$$\sum_{j=0}^p j = [p(p+1)/2] + p + 1$$

(cont'd)

number of arrangements for given k_j (which we postulate to be the relative probability of that value of k_j) is proportional to $\exp[-k_j/(E_1/N^i)]$. The ratio E_1/N^i , which is the average energy per particle, might be called the temperature of the system; and the result shows that any value of k_j has a finite probability, but values of k_j that are very much bigger than E_1/N^i occur very rarely.

Assuming each of these microstates is equally probable, we find that the probability that $k_1 = [(p - j)/p] E_1$ is the number of microstates for that value of k_1 divided by the total number of microstates for all values of k_1 , namely $2(j + 1)/[p(p + 3) + 2]$. Eliminating j by the relation $j = p[(1 - k_1)/E_1]$, we find that the probability of k_1 is

$$P_{3,p}(k_1) = \frac{2(1 - k_1/E_1) + 2/p}{p + 3 + 2/p}$$

A similar argument shows that for $N^i = 4$,

$$P_{4,p}(k_1) = \frac{3(1 - k_1/E_1)[p + (pk_1/E_1) + 3] + 2/p}{(p + 1)(p + 2)}$$

We now convert these expressions (and the corresponding ones for $P_{5,p}$ etc.) into a continuous distribution, taking $dk_1 = E_0$ and letting p go to infinity. The distribution function is then

$$f_{N^i}(k_1) = \lim_{p \rightarrow \infty} \frac{P_{N^i,p}(k_1)}{dk_1} = \frac{(N^i - 1)(1 - k_1/E_1)^{N^i-2}}{E_1} \quad \text{if } k_1 \leq E_1$$

$$= 0 \quad \text{if } k_1 > E_1$$

Recalling the definition, $e = \lim_{y \rightarrow \infty} (1 + y)^{1/y}$ we find that

$$f(k_1) = \lim_{N^i \rightarrow \infty} f_{N^i}(k_1) = (N^i/E_1) \exp[-k_1/(E_1/N^i)]$$

In the more realistic case where the states are equally distributed with respect to momentum rather than energy, the result is

$$f_{N^i}(k_1) = [\Gamma(3N^i/2)/\Gamma(3/2)\Gamma(3N^i/2)] \left[k_1(E_1 - k_1)^{3N^i-5}/E_1^{3N^i-2} \right]^{1/2}$$

$$f(k_1) = \lim_{N^i \rightarrow \infty} f_{N^i}(k_1) = 3 \left[3k_1/2^2(E_1/N^i)^3 \right]^{1/2} \exp[-3k_1/2(E_1/N^i)]$$

The derivation mentioned in the previous paragraph involves an arbitrary assumption about what kinetic energies are allowed; and even though when we take the limit $E_0 \rightarrow 0$ we permit a continuous range of energies, the result is still influenced by the fact that the states of each particle were taken to be uniformly distributed with respect to energy. This is wrong, of course, for according to the laws of physics the states of a free particle (not subject to any forces) are uniformly distributed with respect to momentum. As it happens, both properties are equivalent in two dimensional space, but in three dimensions we do not get the correct energy distribution unless we give each state an additional weighting factor proportional to the square root of its energy (or better, simply sum directly over momentum states). If this correction is inserted into the combinatorial calculation mentioned above*, we find that the probability is proportional to $\sqrt{k_1} \exp -3k_1/2(E_1/N')$ which is in fact nothing but the usual Maxwell velocity distribution. The conventional definition of temperature is $kT = \frac{1}{\beta} = 2(E_0/N')/3$, where k = Boltzmann constant.

The advantage of the canonical ensemble method is that we can treat the energy of each of the N atoms in the system as a random variable independent of the others, as long as N is small compared to N' so that we do not have to worry about energy distributions in which one atom has an energy of the same order of magnitude as E_1 .

We can now apply a standard theorem in probability theory which says that the probability that N random variables have simultaneously a certain set of values is the product of the probabilities for each of these values taken separately, provided that the random variables are independent (i. e., uncorrelated). Hence the relative probability of a microstate of N atoms in which the total kinetic energy is E would be $e^{-\beta E}$ (the so-called "Boltzmann factor" for that microstate). To find the actual numerical value (absolute probability) of this microstate, we have to normalize by multiplying the Boltzmann factor for each state by the number of states having that energy, $g(E)$, and sum or integrate over all possible values of E ; the probability of a microstate with energy E is then given by the formula $p = \frac{e^{-\beta E}}{Z}$ where $Z = \sum g(E) e^{-\beta E}$. The normalizing denominator Z is usually called the partition function (German Zustandszumme, sum-over-states).

*See footnote on pp. 14 and 15.

Up to now we have been dealing only with an ideal gas, so that E is just the kinetic energy of the N atoms, and $g(E)$ is a product of N factors, the square roots of the energies of each atom. The next step is to generalize the above expression for the probability of a microstate, and assert that it is valid when E includes potential-energy terms, corresponding to forces between the atoms or external forces. The justification for this generalization (which is given in detail in textbooks) is that when two or more atoms collide, the total kinetic energy does not necessarily remain the same, but the total energy (kinetic plus potential) is conserved. Hence in statistical equilibrium the probability of a microstate can depend only on its total energy, not on its kinetic energy separately; and in order to make the probability reduce to the correct limiting value when the system becomes an ideal gas (for example when we go to very high temperature or very low density) we must choose the above form.

The grand canonical ensemble represents one further stage of generalization or abstraction; like the canonical ensemble, it can be justified as giving a realistic description of the physical situation even though it appears to be only an artificial model introduced to facilitate calculations. Let us return (in imagination) to the very large system of N' atoms, having fixed energy and fixed volume. Instead of choosing N atoms from this system, suppose that instead we suddenly enclose a volume V with rigid walls and study the statistical properties of the sample of atoms that happen to be trapped in this volume. We assume that the ratio of V to the volume of the original large system is v , and that this ratio also represents the probability that any particular one of the N' atoms is found in the volume V . We ask, what is the probability that there will be exactly N atoms in V , in the limit when N' goes to infinity. v goes to zero, while the product $N'v$ remains equal to a fixed constant? The answer is called the Poisson distribution in statistics or the grand canonical ensemble in statistical mechanics; it is

$$p = A \frac{e^{-\mu N}}{N!} \quad A = e^{-e^{-\mu}} ; \mu = -\log(N'v)$$

It should be noted that the particles have been treated as indistinguishable - permutations of the N particles are not counted as different microstates. If we had assumed that the particles are distinguishable, then the probability that we observe N particles in the volume V could be found by cancelling out the factor $N!$ in the denominator of the above expression and making an appropriate change in the normalization factor A .

Just as the canonical ensemble represents a system that does not have fixed energy but is in equilibrium with a "heat bath" surrounding it at temperature T , so the grand canonical ensemble represents a system (sometimes called an open system) that does not have a fixed number of particles but is in equilibrium with a particle bath surrounding it, characterized by a parameter μ (μkT is usually called the chemical potential).

In many calculations in statistical mechanics, the grand canonical ensemble is used because it allows one to sum over the numbers of particles in different states independently without having to enforce the condition that the total number of particles is fixed. One simply sums over all values of N , or equivalently over all possible values of the numbers of particles in each state; if the result is needed for a particular value of N , rather than for specified volume, the chemical potential μ may be chosen in such a way that the average value of N , viz. \bar{N} , is equal to the specified value. It turns out that when \bar{N} is a large number of the order of magnitude of 10^{22} (as for observable physical systems) the statistical distribution is very sharply peaked at the average value, so that the probability that N differs by more than 0.1 of 1% from \bar{N} is effectively zero.

The grand canonical ensemble is especially useful (and may indeed be the only practical method) for problems involving equilibrium among several kinds of particles, as in an ionized gas. In this case one introduces a chemical potential for each kind of particle, and represents the probability of a state with N_1 particles of Species 1, N_2 of Species 2, and so forth, in the form

$$p = (\text{const.}) \frac{e^{-\mu_1 N_1 - \mu_2 N_2 - \mu_3 N_3 - \dots}}{N_1! N_2! N_3! \dots} g(\Sigma) e^{-\beta E}$$

The constant, which includes the normalizing factor Z from the canonical ensemble and the factor A from the grand canonical ensemble, is found by summing p over all values of $E, N_1, N_2 \dots$ and setting the sum equal to 1; it is also known as the grand partition function (usually without the factor A):

$$Q = \sum_N \frac{Z_N}{N!} .$$

where

$$Z_N = \sum_E g(E) e^{-\beta E}$$

for N particles (with the corresponding generalization for a mixture of several species).

These two partition functions Z and Q , which appeared originally simply as normalizing denominators for the probabilities of states in the ensembles, turn out to be useful quantities themselves, because all thermodynamic properties of the system can be expressed in terms of them. For example, if one differentiates Z with respect to $(-\beta)$, the effect is to multiply each term in the sum by E , and this is the same as finding the average energy for all states in the canonical ensemble:

$$\bar{E} = \sum_E E p(E) = \frac{\sum_E E g(E) e^{-\beta E}}{Z} = \frac{1}{Z} \left(-\frac{dZ}{d\beta} \right) = -\frac{d \log Z}{d\beta}$$

The method sketched above for deriving the probabilities of states by counting microstates may appear to be somewhat artificial, since it was based on assuming a discrete set of kinetic energy states for a free particle and then going to the limit of a

continuous distribution. In the case of classical mechanics, when kinetic energies are not quantized, we could have applied the postulate of equal a priori probability directly to a continuous distribution; this would involve calculating the surface area of a $3N$ -dimensional sphere, corresponding to the region in momentum space for which the total kinetic energy of N particles has a fixed value, and then picking out the part of the surface that corresponds to a particular state (such as velocity of i 'th particle between v_i and $v_i + dv_i$, and so forth). This procedure can be carried out as indicated, and in the limit $N \rightarrow \infty$ it gives a result in agreement with the Maxwell distribution.

However, as soon as one wishes to consider systems in which chemical reactions or ionization processes can change the number of particles, he finds that this approach breaks down; for example, there are infinitely many more possible micro-states for two particles than for one if one assumes a continuous distribution of kinetic energies. It is only by reverting to the description based on a discrete set of states that a reasonable formulation of the equilibrium problem can be found. It turns out that one can derive an equation determining the equilibrium numbers of particles of various species — the Saha equation — provided that the energy unit E_0 is kept finite and not allowed to go to zero. As one might suspect (with the benefit of hindsight) E_0 is closely related to Planck's constant; in fact, one gets the correct physical result by assuming that the size of the elementary cell in phase space is just that indicated by quantum theory. (This discovery, embodied in the Sackur-Tetrode equation for the chemical constant, was one of the triumphs of the old quantum theory.) Thus we see that the theory of ionization equilibrium involves quantum theory and discrete energy states in a very essential way.

The theoretical description of ionization equilibrium for the ideal gas mixture mentioned at the beginning of this section is then as follows: for each ionization process of the type $A_{n-1} \rightleftharpoons A_n + e^-$ (where A_n represents an ion with n electrons removed

from the original neutral atom) the concentrations of these ions in thermal equilibrium are determined by the equation

$$\frac{c_{n-1}}{c_n c_e} = P K^{(n)}(T) \quad (\text{Saha equation})$$

where $c_n = N_n/(N + N_e)$, i.e., the ratio of the number of ions of Type A_n to the total number of particles in the system, including the number of electrons N_e . The ratio for electrons $N_e/(N + N_e)$ is denoted by c_e . P is the pressure, and $K^{(n)}(T)$ is an equilibrium constant (i.e., it is independent of pressure in the ideal-gas approximation) defined as $K^{(n)}(T) = (g_{n-1}/2g_n)(2\pi/m)^{3/2} [h^3/(kT)]^{5/2} \exp(-I_n/kT)$. The symbols in this equation are g_n = degeneracy factor for the ground state of A_n ; likewise for g_{n-1} ; degeneracy factor for electrons is taken as 2 (spin up or down); m = mass of electron; h = Planck's constant divided by 2π ; I_n = n th ionization potential of the atom, usually taken to be equal to the difference in ground state energies of A_n and A_{n-1} . In the form written here it is assumed that all the atoms and ions are in their ground states.

To see how the equation works, we consider the special case of equilibrium between neutral and singly ionized atoms, assuming that the temperature is sufficiently low that the concentration of more than singly ionized atoms is negligible. Then we can define the degree of ionization, α , to be the ratio of the number of singly ionized atoms to the total number of atoms. We have $c = c_1 = \alpha/(1+\alpha)$; $c_0 = (1-\alpha)/(1+\alpha)$ and, after substituting these expressions into the Saha equation and solving for α , we obtain the result $\alpha = 1/[1 + PK^{(1)}]^{1/2}$. Note that (1) the degree of ionization is one (complete ionization) at very low pressures, and decreases to zero as the pressure becomes large; (2) the degree of ionization is one at very high temperatures, and decreases to zero at very low temperatures, but because of the small numerical value of the coefficient of $\exp(-I_n/kT)$ in the formula for $K(T)$, the degree of ionization will be fairly large even for temperatures that are small compared to the ionization energy. Because of this, the number of atoms in excited states will still be fairly small since the excitation energies are usually of the same order of magnitude as the ionization energies.

The Saha equation may be viewed as a special case of the "law of mass action" for chemical reactions, which was established empirically (though without the above definition of K in terms of Planck's constant) before quantum theory. For example, it predicts that an increase in pressure will drive the equilibrium in the direction that leads to a smaller number of particles. Another interpretation, which will be useful in the following sections, is based on the expression for the canonical partition function, $Z = \sum g(E) e^{-\beta E}$, which we now apply to a system containing a fixed number of atoms that may have different degrees of ionization depending on the pressure and temperature. As we showed above, the average energy of the system can be found by differentiating $\log Z$ with respect to $(-\beta)$. It can also be shown that the Helmholtz free energy is $F = -kT \log Z$ which is consistent with the usual thermodynamic relations, $F = E - TS$; $E = -T^2 \left(\frac{\partial F}{\partial T} \right)_V$; $S = - \left(\frac{\partial F}{\partial T} \right)_V$. According to thermodynamics, the Helmholtz free energy F is a minimum for equilibrium at constant volume and temperature; by this is meant that if the system happens to be in any state that is not the equilibrium state, it will tend to go irreversibly toward the equilibrium state and in so doing it will decrease its free energy. The statistical mechanical interpretation of this principle is the following: suppose we group together the possible microstates of a system into a small finite number of macrostates, each of which can be characterized by a certain average energy and entropy; we then write the partition function in the form $Z = Z^{(1)} + Z^{(2)} + Z^{(3)} + \dots Z^{(m)}$; $Z^{(i)} \approx g(E_i) e^{-\beta E_i}$ (we have used an upper subscript in order not to risk confusion with Z_N , which means the complete partition function for N particles). For the sake of concreteness, we may think of each state as being defined by specifying the degree of ionization within certain small limits; thus $Z^{(1)}$ would include all the microstates for which the system is less than 1% ionized, $Z^{(2)}$ includes those with ionization between 1% and 2%, etc. Suppose that at a certain temperature and volume, the largest term in the sum is the one for state i , namely $Z^{(i)}$, then we can write

$$Z = Z^{(i)} \left[1 + \frac{Z^{(1)}}{Z^{(i)}} + \frac{Z^{(2)}}{Z^{(i)}} + \dots + \frac{Z^{(m)}}{Z^{(i)}} \right] = Z^{(i)} S$$

Since by hypothesis $Z^{(i)}$ is larger than any of the others, each term except the first in the brackets will be less than 1; since there are m terms in the sum, the factor in

brackets must be less than m . Hence $\log Z = \log Z^{(1)} + \log S$, where S is less than m . But since m is a small finite number (of the order of magnitude of a few hundred or less) whereas the number of microstates is a very large number of order of magnitude $N!$, we see that $\log Z^{(1)}$, which by Stirling's approximation must be of order $N \log N$, will be extremely large compared to $\log S$. Hence the value of the free energy, $F = -kT \log Z$, will be entirely determined by the corresponding value for that state which has the largest value of $Z^{(1)}$. Although the free energy is really defined only for the equilibrium system as an average over all states, it is useful to imagine that each state has its own free energy, defined as $F_i = -kT \log Z^{(1)}$, and that the thermodynamic properties of the system will be essentially those of the state for which $Z^{(1)}$ is largest, or equivalently, F_i is smallest. In other words, the canonical ensemble contains all states, including those that we would ordinarily call non-equilibrium states, but we can find the equilibrium properties by averaging over all states because the numerical value of any thermodynamic property is almost completely determined by the state that corresponds to equilibrium at the specified volume and temperature. This is the justification for the standard procedure, in statistical mechanics, of replacing the sum over all states by its largest term; it is equivalent to selecting the state with lowest free energy.

In the particular case of an ionized gas, the degree of ionization is simply determined by balancing the energy and entropy in the equation $F = E - TS$. When T is low, the entropy term TS is negligible and one simply looks for the state of lowest energy which in general will be the system of neutral atoms, with all electrons in the ground state. Since the entropy of state i is proportional to the logarithm of the number of microstates in that state [$S_i = k \log g(E_i)$] if we assume as above that $F_i = -kT \log Z^{(1)}$ and $Z^{(1)} = g(E_i) e^{-\beta E_i}$, then it follows that states with a larger number of independent particles will have larger entropy since they have more possible configurations. Hence as the temperature increases and the term TS becomes more important in the free energy, states with more particles (i. e., ionized states) will be favored. At very high temperatures the importance of the energy of each state will be negligible, and only the entropy will count; hence the system will become completely

ionized in order to have the largest possible number of independent particles and the largest number of possible microstates.

It is clear from the above argument that as soon as one knows the free energy for each possible state of the system as a function of temperature and volume, it is possible to determine which will be the equilibrium state at a given temperature and volume by looking for the lowest free energy. In the case of an ideal gas mixture – in which each electron is either bound in its lowest energy level, or free, and interactions between particles are ignored – the process of minimizing the free energy leads to the Saha equation for ionization equilibrium. In the more general case when these assumptions are not permitted, the free energy method still can be used to find the equilibrium composition of the system.

EFFECT OF PARTICLE INTERACTIONS ON IONIZATION EQUILIBRIUM

The standard theory described in the previous section needs to be improved in two important respects before it can be used to calculate occupation numbers in a gas of moderate density. First, a consistent way must be found to calculate the populations of excited electronic states in atoms; and second, the effects of particle interactions must be taken into account. One might think that, in view of the technical difficulties involved in treating particle interactions in systems of medium density, it would be better to postpone the second correction and concentrate on the first one, in the hope that it would at least provide an approximation valid at low densities. Unfortunately this does not seem to be possible, for (at least in the present state of the theory) excited-state populations are closely linked to particle interactions, and one cannot get a reasonable result for the former quantities simply by ignoring the latter.

To illustrate the difficulty in its simplest form, consider the electronic states of the hydrogen atom. According to quantum mechanics, there are an infinite number of energy eigenvalues, which may be divided into two categories: a discrete (but infinite) set of bound states E_n , $n = 1$ to ∞ , and a continuous set of free-particle states with energies $E(\vec{p})$, where the momentum \vec{p} can have any value. The bound state

energies are negative, and are proportional to $1/n^2$ so that they pile up just below zero; the unbound states have positive energies, and are roughly uniformly distributed with respect to momentum except for small energies just above zero. The number of states corresponding to each bound energy level is $2n^2$.

If we applied the canonical ensemble method to calculate the number of atoms in various states of excitation, we would find that all atoms are ionized at any finite temperature, because the continuous infinity of unbound states is (according to the mathematical definition of orders of infinity) of a higher order than the discrete infinity of bound states. If we try to avoid this conclusion by arbitrarily excluding the unbound states and ask for the relative probabilities of the bound levels, we find that the probability that the atom is in its ground state is essentially zero at any finite temperature, because there are an infinite number of excited states. Another way of stating this is to say that the partition function sum is divergent: $Z = 2 e^{-\beta E_0} + 8 e^{-\beta E_0/4} + 18 e^{-\beta E_0/9} + 32 e^{-\beta E_0/16} + \dots = \infty$; hence, the probability that the atom is in its ground state is $p = \frac{1}{Z} (2 e^{-\beta E_0}) = 0$.

The explanation of this paradox is that the set of eigenvalues mentioned above is relevant only for a single hydrogen atom in infinite space, so that the possibility of statistical equilibrium with other particles or a heat bath at some temperature is excluded in principle. As soon as one looks for energy eigenvalues in a slightly different situation - where, for example, the atom is enclosed in a very large but finite box - he finds that there is only a discrete set of free-particle states, not a continuum, and only a finite number of bound states. Of course when the box is very large compared to atomic dimensions, the allowed energies for free-particle states become very densely distributed and almost continuous, and the lower energy levels are almost exactly the same as those for the atom in infinite space. If this were not so, the experimental verification of quantum mechanics by spectroscopy would be much more difficult than it actually is! Nevertheless there is a significant difference between the two cases, finite and infinite volume, and it is especially important for the higher excited states. These are just the states that correspond to charge distributions spread out over the entire volume of the container; the existence of bound states with

infinitesimal binding energy is closely connected with the peculiar long-range character of the Coulomb force law between charged particles. Any type of screening of this force – as might be expected to occur, for example, in an ionized gas – is likely to destroy this long-range character and thereby eliminate the loosely bound excited states.

The central problem in calculating occupation numbers is to find a reasonable and practical way of introducing the effects of particle interactions which will make the partition function, summed over bound states, converge to a finite quantity, hopefully not much larger than the value of the term corresponding to the ground state.

Many different methods for calculating this partition-function cutoff or lowering of the ionization potential have been proposed (Refs. 13 through 25). We discuss here only two of them, which have been selected as being most suitable for the particular problem studied under the contract:

- The Debye-Hückel correction
- The ion-sphere model

The Debye-Hückel correction is based on an approximate evaluation of the effects of electrostatic interactions of charged particles in a plasma or electrolyte solution; it has been extensively used in many other problems, and appears to be quite accurate at low densities and high temperatures. As applied to this problem, it has the effect of increasing the energy of interaction of an electron (charge-e) and a nucleus (charge ze) by an amount $E_{DH} = ze^2/D$ where the Debye length D is defined as

$$D = \left[(4\pi e^2/kT) \sum_i (z_i^2 + z_i) n_i \right]^{-1/2}$$

in an ionized gas consisting of n_i ions of charge $z_i e$. Note that D will be large, and E_{DH} small, when the density is low and the temperature is high. We will discuss the Debye-Hückel correction in more detail in the following subsection; we remark only that it corresponds to taking account of the screening effect in an ionized medium.

which is caused by the tendency for electrons to cluster around ions and thus reduce the effective force exerted by that ion on another charged particle.

The ion-sphere model is the one actually used to obtain our occupation numbers. In this calculation the volume of the gas is divided into sub-volumes, called ion spheres. Each ion sphere contains one ion and, on the average, sufficient free electrons to render it neutral. A state J of the ion sphere is characterized by the number n_J of bound electrons in the ion sphere.

The probability that an ion sphere chosen at random is in the state J is given by the grand canonical ensemble expression $p_J = \exp(-\mu n_J - \beta E_J)/Q(\mu, \beta)$ where $Q(\mu, \beta)$ is the grand partition function. Note that the ensemble is grand with respect to the free electrons only, the number of ions being held fixed. Each ion sphere is treated as if it were a separate thermodynamic system which does not exert any forces on the other ion spheres, but can exchange energy and free electrons with them. The energy E_J is the sum of the bound-free interaction energy and the energy of the bound electrons moving in the field of the nucleus. Thus E_J may be written $E_J = E_J^0 + \lambda n_J$ where λ is the bound-free interaction energy per bound electron. The remainder of the energy, E_J^0 , is assumed to be the same as that of an isolated ion in the same state, and hence is obtainable from spectroscopic data. The values used were those contained in Moore's table (Ref. 11), supplemented by estimates of the missing values.

The value taken for λ is $(3/2)(\bar{n}_f e^2/a)$ where \bar{n}_f is the average number of free electrons per ion sphere and a is the radius of the ion sphere. The details of the method of arriving at this estimate of λ have been described in Ref. 4; another method for deriving it will be indicated in a following subsection. In general it may be said that the model assumes uniform charge density and is based on approximations valid at high densities.

Since the energy change in the ion-sphere model is simply proportional to the number of free electrons, it has the same effect as a change in the chemical potential μ for these electrons in the grand canonical ensemble probability formula. Thus, one can write the probability in the form $p_J = \exp(-\mu_B n_J - \beta E_J^0)/Q(\mu_B, \beta)$ where $\mu_B = \mu + \lambda \beta$.

This is almost the same as the formula for the ideal gas, since the chemical potential μ is only a dummy variable which is determined by the density, and calling it μ_B does not have any significance. The only effect of the energy correction is to eliminate all the bound states whose binding energy is less than λ from the sum over states in Q . This actually requires an iterative procedure, since λ cannot be completely determined until the ion-sphere radius, and hence the density, is known; and the density in turn is not known until one has started with a trial value of μ and calculated the partition function by summing over states. However, in practice the convergence of the iteration is quite fast, so the method is practical.

INTERACTIONS AT LOW DENSITIES; JUSTIFICATION OF THE DEBYE-HÜCKEL CORRECTION

In a gas at very low density, the ionization potential I_n that occurs in the Saha equation is essentially the work that must be done on an electron to remove it to an infinite distance from its bound orbit around a nucleus. In an ionized gas at moderate density, however, the electron is not really being removed to infinity, but only to a distance that is farther from the nucleus than half the average distance between ions in the gas; and its potential energy, when it is free, is not zero as in the previous case, but finite, because it is still being attracted by all the ions in the gas, and repelled by all the electrons. These forces do not balance out to zero, even though there may be an equal amount of positive and negative charge, because the electron is more often found near an ion than near another electron. Hence the work required to remove the electron from the atom is reduced, and the ionization potential is lowered. The actual amount of lowering can be calculated in various ways, leading to different results, and as yet there is no established experimental method that can definitely determine which result is correct. The two methods mentioned previously – Debye-Hückel correction and ion-sphere model – are based on two different views of the interaction of free electrons with ions. The first assumes that the distribution of charge around any given charge is determined by the classical Boltzmann distribution: the positions of both ions and electrons are random, aside from the pre-existing weighting of configurations in which positive charges are surrounded by negative, and conversely. The second method is based on the assumption that the ions are fixed in a regular arrangement in space, and that the electrons in the neighborhood of each ion have a uniform distribution within a sphere, interacting with each other but

not with other electrons or ions. This model is more appropriate to a high-density system, in which the net charge in each sphere averages to zero and fluctuations can be ignored. The actual expression for the energy used in the ion-sphere model can also be derived from quantum mechanics (Ref. 8).

The starting-point for the derivation of the Debye-Hückel correction may be taken to be Poisson's equation for the electrostatic potential,

$$\nabla^2 \phi = -4\pi e \left(\sum_i z_i n_i - n_e \right)$$

where n_e is the electron density,* and n_i is the density of ions of charge z_i . It is assumed that these densities are determined by the electrostatic potential energy ϕ according to the classical Boltzmann distribution, $n_i(r) = n_i(\infty) \exp(-z_i e \phi / kT)$ and a similar equation for n_e : $n_i(\infty)$ and $n_e(\infty)$ are the ion and electron densities at infinite distance from some charge considered fixed at the center; they may also be taken to be the average densities in the system when no charge is considered fixed. The combination of Poisson's equation with the Boltzmann formula for the charge densities is called the Poisson-Boltzmann equation. It should be emphasized that it is not an exact equation, because it is derived from two principles that are valid under different conditions. The Poisson equation applies to a static distribution of charges, whereas the Boltzmann distribution represents the most probable distribution when an average is taken over all microstates in thermal equilibrium at a temperature T . Any one of these microstate distributions, if it were frozen to zero temperature, would satisfy Poisson's equation; but in reality there are rapid fluctuations from one microstate to another in the canonical ensemble, and the Poisson-Boltzmann equation leaves out the effects of these fluctuations. Nevertheless, when treated in the approximate way employed by Debye and Hückel, it happens to give the correct limiting law for the thermodynamic properties at low densities and high temperatures. Debye and Hückel replaced the exponential terms on the right-hand side of the equation by the first two terms of the corresponding power series expansion ($e^{-x} = 1 - x + \dots$). The first

*Here and elsewhere in this section, density means number of particles in unit volume, not mass in unit volume.

term, which is independent of ϕ , is just the total net charge density, which is assumed to be zero; hence the right-hand side of the equation is just proportional to ϕ in this approximation, and the differential equation can easily be solved. The solution which satisfies the correct boundary conditions for an ion of charge ez_i fixed at the origin is $\phi = (ez_i) [\exp(-r/D)/r]$ where D is the Debye length defined above. Thus the effective potential acting on the other electrons and ions looks like a Coulomb potential, ez_i/r , for small distances, but has a screening factor $\exp(-r/D)$ which makes it go rapidly to zero at large distances.

When the Debye-Hückel theory is used to calculate the energy and free energy for an ionic system, it is found that there is a negative term proportional to (e^2/D) for each charged particle. This term can be incorporated into the Saha equation, where it has the effect of a lowering of the ionization potential; likewise it can be used in the occupation number formula, where it has the effect of raising the energy of each bound state and thus bringing it closer to the continuum of unbound states (Refs. 13 and 26 through 29). It should be noted, however, that the correction has no effect on the relative occupation numbers of two low-lying bound states, although it would eliminate entirely some of the upper states by "pushing them into the continuum" of free states.

The effect of the Debye-Hückel correction can also be understood directly from the viewpoint of free energy discussed in the last section. When the Debye-Hückel correction is introduced, it lowers the free energy of the more strongly-ionized states and shifts the equilibrium in the direction of increased ionization.

As mentioned above, the original derivation of the Debye-Hückel correction from the Poisson-Boltzmann equation may not be entirely reliable because the effects of fluctuations have been ignored; moreover, it appears that the expansion of the exponentials and consequent dropping of higher powers of ϕ/kT would lead to serious errors at low temperatures. Indeed, at any temperature the ratio of ϕ to kT would be quite large for small values of r , and one could only hope that such values of r would not contribute very much to the integrals over configurations that must be performed in order to compute thermodynamic properties.

During the last 15 years there have been several attempts* to justify the Debye-Hückel theory on the basis of statistical mechanical principles, and to estimate its accuracy at higher densities and lower temperatures (Refs. 30 through 65). In work performed under the predecessor to this contract, Siegert has studied this question for the purpose of establishing a firm basis for the computation of occupation numbers in an ionized gas (Ref. 6). He considers the gas as a system of ions, neutral atoms, and electrons; the quantum states of the ions and neutral atoms are considered as known, either from experiment or from approximate theoretical calculations. Only those excited states are included for which the mean radius of the charge distribution does not exceed a specified value. The results of the calculations turn out to be independent of the choice of this value within reasonable limits. Electrons are counted as free if they are not included in the ions; this does not of course imply that the interactions between electrons, and between ions and electrons, are neglected. The free electrons are treated classically; this requires that the thermal wavelength $\lambda = h/(2\pi mkT)^{1/2}$ is small compared with the mean distance between electrons and the mean distance between electrons and ions, and thereby imposes a temperature-dependent upper limit on the density for which the calculations are applicable.

The forces between the charged particles are approximated by modified Coulomb potentials, $(1 - e^{-\alpha r})/r$, where α^{-1} is a length parameter of order 10^{-8} cm. Unlike the screened potential that results from solving the Poisson-Boltzmann equation, this is a potential that behaves like a Coulomb potential at large distances, but remains finite at the origin; it is not derived from anything else, but is taken as part of the definition of the model. The introduction of the cut-off serves two purposes: (1) the classical partition function for a system of charged particles with pure Coulomb interaction is infinite, if charges of both signs are present, since there is a possible configuration with infinite negative energy - positive and negative charges at the same point - which makes the Boltzmann factor infinite. Yet if the calculation

*There have been two principal lines of development. The first starts from the observation of J. E. Mayer (Ref. 30) that the well-known cluster integral expansion for the pressure, while apparently divergent for Coulomb interactions, can be rearranged so as to eliminate infinite terms and give the Debye-Hückel correction as a first approximation. The second approach is based on N. N. Bogoliubov's method for describing statistical equilibrium by means of an infinite set of distribution functions, originally published in 1946 (Ref. 38).

is carried through with a finite value of α , it is found that the free energy becomes independent of α at low densities, and α can be taken as small as one wishes.

(2) The calculation with this cr^* -off indicates to what extent the actual deviations of the interparticle forces from the Coulomb law, such as short-range repulsive or attractive forces depending on atomic structure, affect the results. It turns out that short-range forces can be ignored in the low-density ionized gas. The reason is that the energy per particle due to long-range Coulomb forces is proportional to the square root of the density of charged particles — as mentioned above, it is proportional to e^2/D , and D is inversely proportional to the density — whereas the energy due to short-range forces is, at low densities, just proportional to the density since it is proportional to the number of collisions experienced by a particle. Hence the ratio of the energy of short-range forces to that of long-range forces is proportional to the square root of density, and must go to zero as the density goes to zero.

Siegert (Ref. 6) has shown that the results previously established for the free energy of ionized systems can be directly applied to yield a formula for occupation numbers. He has also examined the validity of the Debye-Hückel approximation by expressing the canonical ensemble partition function in terms of collective coordinates, and applying the central limit theorem of probability theory. The result is that the Debye-Hückel correction is valid provided that the condition $[(6)^{1/3}/(2\pi)^{5/3}][(V/N)^{1/3}/D] \ll 1$ is satisfied, where N is the number of charged particles in volume V . This is a more quantitative way of stating the condition that the geometric mean distance between particles must be small compared with the Debye length D .

In Appendix A (Sec. A. 1), DeWitt has generalized Siegert's theory of occupation numbers by using the grand canonical ensemble. There are at least two reasons why this generalization is useful. First, by using the grand canonical ensemble it is easy to include quantum-mechanical electron degeneracy effects. Second, results for the interaction free energy including quantum effects for a dense plasma are usually obtained using the grand partition function.

Since we will also need the quantum-mechanical expression for the electron distribution function when we discuss the basis for the ion-sphere model, it seems worthwhile to review its derivation at this point.

Assume we have a grand canonical ensemble of systems of electrons, characterized by a temperature T and a chemical potential μ . Each electron may have one of an infinite number of possible energies, which we call E_0, E_1, E_2, \dots (this is a discrete, not a continuous, set of numbers). No two electrons may have the same energy;* but aside from this "exclusion effect" there is no interaction between the electrons. The number of electrons that have energy E_k will be called n_k ; and by our hypothesis, $n_k = 0$ or 1 . The total energy of any particular microstate of n electrons is then $E = n_0 E_0 + n_1 E_1 + \dots$; $n = n_0 + n_1 + n_2 + \dots$. The probability of this microstate is assumed to be given by the expression quoted for classical systems in the second subsection, provided that none of the n_k is greater than 1 , but is otherwise zero: $p(n_0, n_1, \dots) = Ce^{-\mu n - \beta E}$ where C is a constant to be determined by summing this expression over all values of all the n_k , and setting the sum equal to 1 . As usual, the chemical potential μ is to be chosen so as to make the average value of n come out equal to the desired value.

We now ask, what is the probability that there are n_k electrons with energy E_k , regardless of the number of electrons with other energies? This probability is found simply by summing the above expression for p over all energies except E_k :

$$P(n_k) = \frac{C \sum e^{-\mu n - \beta(n_0 E_0 + n_1 E_1 + \dots)}}{C \sum e^{-\mu n - \beta(n_0 E_0 + n_1 E_1 + \dots)}}$$

*This assumption is made only to illustrate the method of derivation, the case when the maximum number of electrons with a given energy is a small finite number can be treated in a similar manner.

where the prime on the upper sum means that all values of all n 's except n_k are to be summed over, whereas in the lower sum all values of all n 's are included. It is easily seen that the primed sum is also a factor in the unprimed sum and thus cancels out, so that we get

$$P(n_k) = \exp [-(\mu + \beta E_k) n_k] / \sum_{n_k} \exp [-(\mu + \beta E_k) n_k]$$

Since n_k is permitted to have only the values 0 and 1, this reduces to $P(n_k) = \exp [-(\mu + \beta E_k) n_k] / 1 + \exp [-(\mu + \beta E_k)]$. The average value of n_k can now be calculated: it is

$$\bar{n}_k = \sum_{n_k} n_k P(n_k) = 0P(0) + 1P(1) = \exp [-(\mu + \beta E_k)] / \{1 + \exp [-(\mu + \beta E_k)]\} = 1 / (1 + \exp (\mu + \beta E_k))$$

The above derivation was based on the assumption that no two electrons may have exactly the same energy. If instead it is possible for as many as g_k electrons to have the same energy, the same argument still applies and the result for \bar{n}_k is simply multiplied by g_k (for example, $g_k = 2$ if the electrons can have spins up or down). In order to use this general formula for \bar{n}_k it is necessary to know what the allowed energies E_k are, and then to evaluate the sum over all microstates in order to find the relation between μ and the density. It is usually necessary to approximate the sum by an integral for this purpose. It can be shown by solving the Schrödinger equation that the number of states of a free electron without spin in a container with volume V , corresponding to energies between E_k and $E_k + dE_k$, is $(4\pi v/h^3)m\sqrt{2mE_k} dE_k$. Thus we can calculate approximately the average value of any quantity that depends on the energies of the electrons, $F(E)$, by using an integral of the form

$$\bar{F}(E) = (4\pi v/h^3)m\sqrt{2m} \int_0^{\infty} \frac{f(E)E^{1/2} dE}{1 + \exp(\mu + \beta E)}$$

In particular, the total number of electrons in all states is found by setting $f(E) = 1$:

$$n = (4\pi v/h^3)m\sqrt{2m} \int_0^\infty \frac{E^{1/2} dE}{1 + \exp(\mu + \beta E)}.$$

We can regard this as an equation giving μ as a function of n , even though there is no simple solution of the equation except for the special case of zero temperature; usually we have to find μ by numerical calculation or by expansion in power series.

For calculations with the quantum-mechanical electron gas it is convenient to define the set of functions

$$I_m(\alpha) = \{1/\Gamma(m+1)\} \int_0^\infty \frac{(dz)z^m}{1 + \exp(z - \alpha)}.$$

These are standard functions that have been extensively studied and tabulated; however, the notation and definitions vary somewhat with different authors.

We now return to DeWitt's theory of occupation numbers which takes account of quantum effects as well as interactions between charged particles.

To illustrate a few points that will come up in the treatment of a multicomponent ionized gas, we first look at the electron gas in a continuous background of positive charge. The background is needed to ensure electrical neutrality of the system but does not play any other role in the calculation. The grand partition function is

$$Q = \sum_{N, E} \exp(\mu N - \beta E).$$

We define the thermodynamic potential Ω by the relation $Q = e^{\beta\Omega}$. It can be shown that Ω is equal to the product of pressure and volume for the system, where the

pressure is expressed as a function of the chemical potential μ . The average energy and average number of particles may be found by differentiating $\beta\Omega$ with respect to β and μ , respectively:

$$\bar{E} = -\frac{\partial(\beta\Omega)}{\partial\beta} = \frac{\sum E \exp(\mu N - \beta E)}{\sum \exp(\mu N - \beta E)}$$

$$\bar{N} = \frac{\partial(\beta\Omega)}{\partial\mu} = \frac{\sum N \exp(\mu N - \beta E)}{\sum \exp(\mu N - \beta E)}.$$

For the electron gas with interactions, we may write the thermodynamic potential as

$$\Omega = \bar{N} \frac{I_{3/2}(\mu)}{\zeta} + \Omega_{\text{int}}$$

where

$$\zeta = \frac{h^3(\bar{N}/V)}{2\pi^{3/2}(2mkT)^{3/2}} = I_{1/2}(\mu_0).$$

The first term represents the value for the ideal quantum gas without interactions, and the second term (as yet undetermined) represents the effect of interactions. Similarly we may write the chemical potential as the sum of its ideal-gas value and a correction term for interactions, $\mu = \mu_0 + \delta\mu$. We now substitute this into the above expression for \bar{N} and make a Taylor expansion in powers of $\delta\mu$, dropping terms involving second or higher powers of $\delta\mu$. It is then found that, when the interactions can be treated as a small perturbation, the shift in chemical potential is

$$\delta\mu = -\frac{\partial(\beta\Omega_{\text{int}})}{\partial N}$$

Classical Coulomb-interaction effects in the electron gas are functions of the dimensionless parameter $A = \beta e^2/D = 2\pi^{1/2} e^3 \beta^{3/2} \bar{N}/V$. In the grand partition function the corresponding quantity is $A e^{\delta\mu/2}$ because everywhere N appears it should be replaced by $\bar{N} e^{\delta\mu}$. The Helmholtz free energy for the classical electron gas is (Refs. 32, 34, 37, and 40)

$$\beta F = \bar{N} \left[(\mu_0 - 1) - \left[\frac{\Lambda}{3} + \frac{\Lambda^2}{12} \left(\log 3\Lambda + 2C - \frac{11}{6} \right) \right] \right] + (\text{terms of higher order in } \Lambda) \quad (C = \text{constant}).$$

The Debye-Hückel correction appears as the term $-\bar{N} \frac{\Lambda}{3}$ in this expression. For this case the correction to the thermodynamic potential is found to

$$\delta\mu = -\frac{\Lambda}{2} - \frac{\Lambda^2}{6} \left(\log 3\Lambda + 2C - \frac{19}{12} \right).$$

For the more realistic case of a multicomponent ionized gas the same analysis can be carried through for the ion-ion and electron-electron interactions, but for the attractive ion-electron interactions one has to start out with some kind of short-range cut-off, or else include quantum effects, in order to exclude configurations with ions sitting on top of electrons. Which approach is chosen will depend on the extent of theoretical progress in evaluating the quantum effects at the time the numerical calculation is actually undertaken; it is expected that a good quantitative estimate of the quantum-mechanical free energy for electron interactions will be obtained fairly soon. The following treatment is general enough to permit the use of any exact or approximate expression for these interactions which may be available.

We consider a gas composed of N_i nuclei of charge Z and ZN_i electrons. At low-enough temperatures the gas will consist merely of N_i neutral atoms; at very high temperatures it will be completely ionized. At intermediate temperatures every ionic species is possible; we characterize a state of the system by the number of free electrons, n_e , and the number of ions of charge z , n_z ($z = 0$ to Z). The quantum numbers for the internal energy states of an ion of charge z will be denoted collectively as J_z : the number of such ions in state J_z will be called n_{z,J_z} , and the energy levels will be denoted $\epsilon(z, J_z, n_e, \{n_z\})$. These levels are functions of the numbers of various kinds of charges because the energy levels of the ion in a vacuum [denoted by $\epsilon^0(z, J_z)$] will be shifted upward due to screening by other charges in the plasma. If one assumes that the least-bound electron on an ion of charge z moves in a Coulomb field corresponding to a central charge $z + 1$ (nucleus and core of ionized electron), but with this Coulomb field screened according to the Debye-Hückel theory, so that the effective potential is $-(z + 1)(e^2/r) \exp(-r/D)$, then the

energy levels will be: $\epsilon(z, J_z, n_e, \{n_z\}) = \epsilon^0(z, J_z) - (z+1)e^2/D + \delta\epsilon(J_z, n_e, \{n_z\})$ where the vacuum levels will be hydrogenic, the second term is a constant energy shift upward for all levels, and the third term will be, in lowest approximation, the difference between the Debye screened potential and the original Coulomb potential, averaged over the charge distribution of J_z . It is assumed here that the energy of the level is measured from the vacuum continuum limit. Actually, however, the continuum limit for electrons is effectively lowered by the amount $-e^2/D$. Thus bound levels above this lowered continuum limit find themselves no longer bound. The number of states to be counted as bound is determined by the condition that: $\epsilon(z, J_z, n_e, \{n_z\}) + e^2/D < 0$.

As Siegert (Ref. 6) showed, the probability of a state with n_e free electrons and the set $\{n_{z,J}\}$ of occupation numbers for the ions is

$$p(n_e, \{n_{z,J_z}\}) = \frac{\left(\frac{2V}{\pi^{-3/2}\lambda_e^3}\right)^{n_e} \prod_z \left[\frac{(2s_z + 1)V}{\pi^{-3/2}\lambda_1^3}\right]^{n_z}}{n_e! \prod_{z,J_z} n_{z,J_z}!} \times \exp \left[-\beta F_{\text{int}} - \beta \sum_{z,J_z} n_{z,J_z} \epsilon(z, J_z, n_e, \{n_z\}) - n_0^2 b_2(3)/V \right]$$

where $\lambda_e = h/(2m_e kT)^{1/2}$, $\lambda_1 = h/(2m_1 kT)^{1/2}$, s_z = spin of ion with charge z . The term F_{int} in the exponential is the Coulomb free energy due to the interaction of free electrons and ions, which is just the Debye-Hückel correction if the density is sufficiently low,

$$\beta F_{\text{int}} \approx -\frac{\beta}{3} \left(n_e + z^2 n_z \right) \frac{e^2}{D} = -\frac{1}{3} \frac{V}{4\pi D} \beta$$

The last term in the exponential is the effect of short-range forces, which here is the second-virial-coefficient approximation.

This result could be improved by treating the ions as extended structures rather than as points, perhaps by describing the bound electrons with some kind of form factor. Also, it could include the electrostatic free energy terms of order Λ^2 mentioned above, (Refs. 32, 34, 37, and 40) which can be generalized to multicomponent systems although a cutoff is required for the ion-electron interactions. A consistent quantum-mechanical treatment of these interactions would have to include both bound and scattering states of the electron, so that the separation of the total energy into distinct contributions from free and bound electrons which is implied by the above formula may not be exactly correct.

From this expression for p , we wish to find the most probable state, subject to the condition of electrical neutrality, $n_e = \sum z n_z$. This can be done with a slight modification of the grand canonical ensemble method, or equivalently by the method of Lagrange multipliers. We introduce two multipliers, α_i and α_e , and determine the state for which the quantity $L = \log p + \alpha_i \sum n_z + \alpha_e (n_e - \sum z n_z)$ is stationary. The result is that the average occupation numbers are

$$\bar{n}_e = \frac{2\pi^{3/2} V}{\lambda_e^3} \exp \left\{ \alpha_e - \frac{\partial \beta F_{\text{int}}}{\partial n_e} - \beta \sum_{z, J_z} \bar{n}_{z, J_z} \frac{\partial \epsilon}{\partial n_e} \right\}$$

$$\begin{aligned} \bar{n}_{z, J_z} = & \frac{(2s_z + 1)\pi^{3/2} V}{\lambda_i^3} \exp \left\{ (\alpha_i - z\alpha_e) - \frac{\partial \beta F_{\text{int}}}{\partial n_z} - \beta \epsilon(z, J_z, n_e, \{n_z\}) \right. \\ & \left. - \beta \sum_{J_z} \bar{n}_{z, J_z} \frac{\partial \epsilon}{\partial n_z} - 2\beta \bar{n}_0/V b_2(\beta) \delta_z \right\} \end{aligned}$$

The equation for \bar{n}_{z, J_z} contains two terms not present in Siegert's expression, namely that containing $\frac{\partial \epsilon}{\partial n_z}$, which takes into account the possible density dependence of the energy levels, and the term involving the second virial coefficient $b_2(\beta)$ for interaction between neutral atoms (note that the Kronecker symbol δ_z is 1 if $z = 0$ and 0 otherwise). The equations are not explicit expressions for the

occupation numbers, since the occupation numbers themselves appear in the exponents on the right-hand sides, and also since the chemical potentials α_i and α_e have not yet been determined as functions of density. This determination requires summation over all occupation numbers for different states of each ion; but the number of states to be included in the sum will in turn depend on the amount of lowering of the ionization potential and hence on the composition of the system. Just as in the ion-sphere model, an iterative procedure is needed. One possible scheme, which has not yet been tried out in practice, is to use the following expression for the average ionic charge \bar{z}

$$\bar{z} = \frac{\sum_z z \bar{n}_z}{\sum_z \bar{n}_z} = \frac{\sum_z z \sum_{J_z} n_{z,J_z}}{\sum_z \sum_{J_z} n_{z,J_z}}$$

and express α_e in terms of the chemical potential in the absence of interactions, α_{e0} , and the corrections for interactions:

$$\alpha_e = \alpha_{e0} + \frac{\partial F_{int}}{\partial n_e} + \beta \sum_{z,J_z} \bar{n}_{z,J_z} \frac{\partial \epsilon}{\partial n_e}$$

where

$$\alpha_{e0} = \log t_e = \log \frac{\hbar^3 (\bar{z} N_i / V)}{2 \pi^{3/2} (2 m k T)^{3/2}}$$

One can guess a value for \bar{z} , then compute α_{e0} and α_e and substitute these values into the equation for n_{z,J_z} to determine a new value of \bar{z} , continuing until convergence is attained.

Quantum effects for the electrons can be included in this scheme, using the grand canonical ensemble; the thermodynamic potential is

$$\beta \Omega = \log Q = \bar{n}_e \frac{1/2(\alpha_e)}{t_e} + \frac{\bar{N}_i}{\xi_i} \sum_z (2s_z + 1) \exp(\alpha_i - z\alpha_e - \beta f_z) + \beta \Omega_{int} + \alpha_e^2 \bar{n}_e^2 / V$$

where f_z is defined in terms of the partition function for an ion of charge z :

$$e^{-\beta f_z} = \sum_{J_z} e^{-\beta \epsilon(z, J_z, n_e, \{n_z\})}.$$

An equation for \bar{x} , generalizing the one given above for the classical case, has also been obtained; it can be solved by a similar iterative procedure to get occupation numbers, valid at high densities, if Ω_{int} is known.

Another effect which should be included is the shift of bound-state energy levels due to screening of the interaction between the nucleus and the orbital electron by other charged particles in the system. The magnitude of this effect can be estimated by the following argument (Appendix A): assume that we have decided how many levels are to go into the calculation of f_z , either by taking the last one under the lowered continuum, or perhaps the last distinct line before broadening merges the remaining upper levels. Suppose further that we can calculate these levels by solving the Schrödinger equation with the screened Debye potential, $(z+1)(e^2/r)e^{-r/D}$. Suppose further that the resulting energy levels may be written as an expansion in powers of $(a_0/D)/(z+1)$ since the Bohr radius for the core charge $z+1$ is $a_0/(z+1)$:

$$\epsilon(z, J_z, n_z, \{n_z\}) = -\frac{(z+1)^2}{n^2} \text{ rydbergs} + (z+1)(e^2/D) - a_{1,z,J_z} \frac{e^2 a_0^2}{D^2} + a_{2,z,J_z} \frac{e^2 a_0^2}{D^3} + \dots$$

where the coefficients a_{n_1, n_2, n_3} are numbers to be calculated from the multipole matrix elements, $\langle r^{\pm} / a_0^{\pm} \rangle$. Presumably if these energy levels are fed into the calculation of f_z , then f_z could also be written as such an expansion:

$$f_z = f_z^{(0)} + (z+1) \frac{e^2}{D} - b_{1,z} \frac{e^2 a_0^2}{D^2} + b_{2,z} \frac{e^2 a_0^2}{D^3} - \dots$$

The terms in the chemical-potential shifts depending on the energy levels can be estimated, and we can conclude that at low densities for which $a_0 \ll D$, only the first term of the energy shift should be sufficient to give an accurate result:

$$\beta n_z \frac{\partial f_z}{\partial n_z} + z \beta n_e \sum_{z'=0}^{z-1} \frac{\partial f_{z'}}{\partial n_e} = \frac{\beta e^2}{2D} \frac{(z+1)z^2 n_z + z n_e z(z+1)/2}{\sum z^2 n_z + n_e}.$$

It appears that this result could be of the same order as the shift obtained from the Debye-Hückel free energy. This effect will have to be investigated before extensive calculations with the electrostatic free-energy corrections are undertaken. A study of this effect in hydrogen has been carried out from another direction (under the present contract). This has been reported in the open literature (Ref. 66) and, hence, will not be discussed here.

INTERACTIONS AT HIGH DENSITIES; DISCUSSION OF ION-SPHERE MODEL

According to the theory of ionization-potential lowering by electron interactions – which we may call "pressure ionization" for brevity – electrostatic effects tend to encourage ionization at low densities and high temperatures. Since these electrostatic effects increase with density, it is conceivable that at some point they could outweigh the usual effect of pressure, which is to suppress ionization. Thus we might observe that the degree of ionization first decreases with pressure (as the Saha equation predicts), then reaches a minimum and starts to increase with pressure. This is indeed what would happen if the Debye-Hückel correction were applicable in its usual form at high pressures, and one would thus have "pressure ionization" due to a purely classical electrostatic effect, even if no account were taken of quantum effects or shifts of electronic energy levels (Refs. 26, 67, and 68). Actually this cannot happen in general, for the Debye-Hückel theory does not give an accurate estimate of the classical electrostatic effects at higher densities, as can be seen from the fact that it predicts that the total pressure of an ionic mixture at fixed composition will become negative at high densities. When the Debye-Hückel theory is corrected by using the results of recent statistical mechanical theories (Refs. 30 through 65), together with a short-range cutoff on the Coulomb potential, the difficulty of negative pressure is avoided, and it is found that except in rather special cases the predicted minimum in

the ionization vs. pressure curve occurs at a pressure so high that the theory is probably not valid (Ref. 69). Unfortunately most of the theoretical treatments of the classical ionized gas are based on power series expansions starting from the low-density high-temperature limit, and cannot be expected to give reliable results at high densities and low temperatures; moreover, it is just in the latter region that quantum effects cannot be ignored. We must therefore leave open the question of the behavior of the hypothetical classical ionized gas at high densities, and turn to another model which is more realistic though harder to treat in a systematic theoretical way.

It seems to be fairly well established, by a combination of theoretical and experimental studies, that all matter will be completely ionized at sufficiently high densities; and that even at moderate densities and temperatures the effect of interactions of neighboring particles on an atom will be to "iron out the details of electronic structure that are responsible for the characteristic "chemical" differences between atoms with different nuclear charges. For this reason, it is frequently useful to treat the electrons in an atom as if they formed an "ideal quantum gas" in which interactions are ignored except for the assumption that the density at each point is determined by the electrostatic potential at that point. This is the well-known Thomas-Fermi model of the atom. It is somewhat similar to the Debye-Hückel theory, in that it starts by assuming that the electrostatic potential is determined by Poisson's equation,

$$\nabla^2 \phi = -4\pi e \left(\sum_i z_i n_i - n_e \right)$$

where n_e is the electron density, and n_i is the number density of ions of charge z_i . But now, instead of assuming that both n_e and n_i are related to ϕ by the Boltzmann formula of classical statistical mechanics, we use the Boltzmann formula only for the ions, and insert the appropriate quantum-mechanical expression for the electron density,

$$n_e(r) = n_e(-\alpha) \frac{1}{r} \left[\frac{e\phi(r)}{kT} - \alpha \right] / F(-\alpha)$$

where

$$F(\eta) = \int_0^\infty \frac{t^{1/2} dt}{1 + \exp(t - \eta)}$$

The degeneracy parameter, α , is determined by the equation

$$n_e(\infty) = [2(2\pi mkT)^{3/2}/h^3] [2F(-\alpha)/\sqrt{\pi}] .$$

For the region of moderately high densities, with which we are concerned, α is always positive and appreciably larger than 1, and we can use the approximation $2F(-\alpha)/\sqrt{\pi} \approx e^{-\alpha} \ll 1$. Essentially this means we are assuming that the free electrons are nondegenerate, i.e., quantum effects are small for them. Close to the nucleus, where $e\phi > \alpha kT$, there is a region of degenerate bound electrons, the ion core.

Following Stewart and Pyatt (Ref. 8), we can write the Thomas-Fermi equation for the ionized gas in the form

$$\frac{1}{x} \frac{d^2}{dx^2} (xy) = \frac{1}{z^* + 1} \left[\frac{F(y - \alpha)}{F(-\alpha)} - \frac{\langle z e^{-zy} \rangle}{\langle z \rangle} \right]$$

where $y = e\phi/kT$, $x = r/D$, and D is the Debye length; the symbol $\langle \rangle$ means an average over ionic species using the density $n_i(\infty)$, and $z^* = \langle z^2 \rangle / \langle z \rangle$. The total electrostatic potential ϕ is then separated into two parts, the potential due to a nucleus considered fixed at the origin, and a perturbing potential produced by free electrons and neighboring ions. The perturbing potential ϕ_f satisfies a similar equation in which only the free-electron and ion densities appear (Ref. 8):

$$\frac{1}{x} \frac{d^2}{dx^2} (xy) = \frac{1}{z^* + 1} \left[\frac{F(y - \alpha, y)}{F(-\alpha)} - e^{-z^* y} \right]$$

where

$$v = e\phi_f/kT; F(y - \alpha, y) = \int_y^{\infty} \frac{t^{1/2} dt}{1 + \exp(t + \alpha - y)}.$$

For large values of x , where $y \ll 1/z^*$, the equation for y reduces to the Poisson-Boltzmann equation, which has the usual Debye-Hückel solution $y = \frac{C}{x} e^{-x}$. In this region the charge densities of ions and electrons nearly cancel and most of the electrons are free. For smaller values of x , if $z^* \gg 1$, there is a region where $1/z^* \ll y \ll 1$, and the density of the ions and that of the bound electrons are small compared with that of the free electrons, the latter being approximately constant and equal to its asymptotic value $n_e(\infty)$. In this region the equation for y is approximately (Ref. 8)

$$\frac{1}{x} \frac{d^2}{dx^2} (xy) = \frac{1}{z^* + 1}$$

which has the solution $y = \frac{A}{x} + B + \frac{x^2}{6(z^* + 1)}$ where A and B are constants. For even smaller values of x , most of the electrons are bound, and the solutions are those of the usual Thomas-Fermi theory. If we ignore this inner region and construct an approximate solution for the two outer regions, having the form

$$y = \begin{cases} \frac{C}{x} e^{-x} & \text{for } x > x_1 \\ \frac{A}{x} + B + \frac{x^2}{6(z^* + 1)} & \text{for } x < x_1 \end{cases}$$

requiring that y and dy/dx be continuous at x_1 , we find that the constants must be related by the equation (Ref. 8) $-2(z^* + 1)B + 1 = [3(z^* + 1)A + 1]^{2/3}$. Now define the ion-sphere radius a for an ion of charge z by the condition

$$\frac{4\pi a^3}{3} = \frac{z}{n_e(\infty)}.$$

It is then found that when the ratio $\frac{a}{D}$ is small (low density, high temperature) the relation between the constants reduces to $A = -B = ze^2/DkT$ and the electrostatic potential is the same as the Debye potential; when $\frac{a}{D}$ is large, A is also large, but $-B$ reduces to $-B = 3ze^2/2akT$ which is equivalent to the result of the ion-sphere theory. Thus the Stewart-Pyatt theory provides a justification for the ion-sphere model by deriving it as an approximate solution of the Thomas-Fermi model, valid at moderately high densities and low temperatures, and at the same time showing how the same basic model can lead to the Debye-Hückel correction at low densities and high temperatures.

The Thomas-Fermi model itself is of course only an approximation which is inaccurate except at very high densities. In recent years there has been a large amount of research on the quantum-mechanical electron gas (Refs. 70 through 76), as well as some attempts to deduce the Thomas-Fermi model as the first approximation in a systematic power series expansion starting from the high-density limit (Refs. 77 and 78). Since it is expected that this research will eventually lead to results that will be useful in calculating occupation numbers of ionized gases at high densities, we shall summarize here what is now known about the free energy of a multicomponent plasma. See Appendix A (Sec. A.2) for the details. These remarks apply mainly to the case of high temperatures, where the Debye-Hückel term with quantum-mechanical "diffraction" corrections is the dominant Coulomb interaction contribution, and is proportional to the square root of the density. We shall discuss the next term after this, which gives a contribution to the free energy proportional to $\rho \log \rho$.

For simplicity we begin with a discussion of a one-component plasma, the electron gas in a continuous positive background which is included only to ensure electrical neutrality. The state of such a plasma can be described in terms of three fundamental length parameters:

$$\begin{aligned}
 L &= \frac{ze^2}{D} = \text{distance of closest approach} \\
 \lambda &= \frac{\hbar}{(2mkT)}^{1/2} = \text{thermal DeBroglie wavelength} \\
 D &= (4\pi\beta e^2 \rho)^{-1/2} = \text{Debye screening length}
 \end{aligned}$$

The three possible ratios of these lengths give the dimensionless parameters which are useful for writing down formulae for the free energy, namely:

$$\text{Classical plasma parameter, } \Lambda = L/D = 2\pi^{1/2} e^3 \beta^{3/2} \rho^{1/2}$$

$$\text{Quantum diffraction parameter, } \gamma = \lambda/D = (2\pi)^{1/2} \hbar c \beta \rho^{1/2} m^{-1/2}$$

$$\text{Wigner-Kirkwood expansion parameter, } \eta = \lambda/L = \gamma/\Lambda = 2^{-1/2} \hbar c^{-2} \beta^{-1/2} m^{-1/2}$$

At high temperatures the three lengths may be ordered in the sequence $L < \lambda < D$ and hence the dimensionless parameters satisfy the relations $\Lambda < \gamma < 1$, $\eta < 1$. This is the limit in which we wish to give a correct result for the free energy of the multicomponent system. "High temperature" here means that kT is greater than 1 rydberg; when this is true, the thermal wavelength is greater than the distance of closest approach, and consequently quantum-mechanical diffraction effects must have some residual importance.

It is possible to evaluate the free energy of a low-density classical electron gas ($\hbar = 0$) following Meeron, Friedman, and Abe (Refs. 32, 34, and 37). Also, by using the Wigner-Kirkwood expansion (Refs. 79 and 80) one may estimate first-order quantum corrections due to the uncertainty principle (i. e., "diffraction" effects but not "statistics" effects). For the Coulomb potential the Wigner-Kirkwood expansion parameter is η as defined above. This parameter becomes large at high temperatures, and consequently the Wigner-Kirkwood expansion for the Coulomb potential can only be valid in the low temperature limit ($\eta < 1$). This situation is to be contrasted with the application of the Wigner-Kirkwood expansion to ordinary non-ideal gases with short-range intermolecular forces (for example, a Lennard-Jones interaction) where the expansion parameter becomes small at high temperatures. The Wigner-Kirkwood expansion for various force laws has been discussed by DeWitt (Ref. 81): the result for the electron-gas free energy at low temperature is $\beta(F - F_0)/N - \frac{\Lambda}{3} - \frac{\Lambda^2}{12} (\log \Lambda + \text{constant}) \dots + \Lambda^2 f(\eta^2)$ where $f(\eta^2) = -\frac{\eta^2}{12} + \frac{\eta^4}{60} + \frac{\eta^6}{63} + \dots$ and F_0 is the ideal-gas free energy. (Recall that $\frac{\Lambda}{3}$ is the Debye-Hückel term.) For this result to be valid, the fundamental length parameters must be ordered as follows: $\lambda < L < D$ and the dimensionless parameters as $\gamma < \Lambda < 1$, $\eta < 1$ ($kT < 1$ rydberg).

One might ask whether this limit makes any sense, since for real electrons the effect of Fermi statistics as well as diffraction must be considered at low temperatures. The answer is that the effects of statistics are important, but it is more convenient to treat them separately by a different method; for the purposes of the present discussion we shall exclude them (somewhat artificially) by the device of giving the electrons a large spin s . The gas remains nondegenerate, and has a nearly Maxwellian velocity distribution, as long as $\xi = \frac{\rho\lambda^3}{2s+1} \ll 1$. The gas is partially degenerate when $\xi \sim 1$, and very degenerate when $\xi \gg 1$.

The function $f(\eta^2)$ represents the sum of the entire Wigner-Kirkwood series, of which only the first three terms have been calculated. Although it would be very difficult to calculate any further terms in this series, it is possible to obtain the asymptotic value of $f(\eta^2)$ for large η , which is what we need for the high-temperature case (Ref. 82):

$$f(\eta^2) \underset{\eta \gg 1}{\longrightarrow} \frac{\pi^{1/2}}{2^{7/2}} \eta - \frac{1}{12} \log \eta.$$

The high-temperature free energy is then

$$\beta(F - F_0)/N = -\frac{\Lambda}{3} \left(1 - \frac{3\pi^{1/2}}{2^{7/2}} \gamma + \dots \right) - \frac{\Lambda^2}{12} (\log \gamma + \text{constant}) + \dots$$

for $L < \lambda \ll D$, i.e., $\Lambda < \gamma < 1$ and $\eta > 1$. It should be noted that the "constant" in this equation has not yet been calculated.

The exchange corrections in the high-temperature limit have the form

$$\frac{1}{2s+1} \left\{ \frac{1}{2} \gamma^2 - \frac{\pi^{1/2} \log 2}{2^{5/2}} \gamma \Lambda + (\text{constant}) \Lambda^2 + \dots \right\}.$$

The constant in this equation is different from the previous one but is likewise not yet known.

We may now write the result for the free energy of the multicomponent plasma at high temperatures, using the above-mentioned results. In a two-component plasma there is an additional parameter, the electron-ion mass ratio m_e/m_i . There will now be three de Broglie wavelengths, corresponding to electron-electron, electron-ion, and ion-ion interactions. In real plasma the ion mass is at least 1836 times the electron mass, and this fact has an important effect on the logarithmic term in the free energy. In the temperature region defined by $1 \text{ rydberg} < kT < (m_i/m_e) \text{ rydbergs}$, the lengths of the two component system are arranged in the order $\lambda_{ii} < L < \lambda_{ee}$
 $\approx \lambda_{ei} \ll D$, where

$$\lambda_{ei} = \hbar/(2\mu kT), \quad \mu = \frac{m_e m_i}{(m_e + m_i)}.$$

The result for the free energy is then

$$\beta(F - F_0)/N = -\frac{\Lambda}{3} - \frac{\Lambda^2}{12} \left\{ f_e^2 \log \frac{\lambda_{ee}}{D} - 2z_i^3 f_e f_i \log \frac{\lambda_{ei}}{D} + z_i^6 f_i^2 \log \frac{\beta e^2}{D} \right\}$$

where $f_e = \rho_e/\rho$, $f_i = \rho_i/\rho$, $\rho = \rho_e + \rho_i$; z_i = ionic charge. Diffraction and exchange corrections have not been included here because we are looking mainly at the logarithmic terms. Note that if the temperature is $kT > (m_i/m_e) \text{ rydbergs}$, the ion-ion interaction terms would become $\log(\lambda_{ii}/D)$. Also, if the electrons and ions have equal and opposite charge and the same mass, the logarithms in this expression would all be equal, and the bracket term would be zero. This hypothesis is, of course, untrue (except for ionized positronium!) and for real ionized gases the above results depend strongly on the electron and ion masses.

It should be noted that the above result can be obtained by relatively simple calculations because the temperature has been assumed to be so high that the gas is fully ionized; furthermore, third-order perturbation theory is sufficiently accurate because the thermal wavelength is greater than the distance of closest approach. When these conditions are not fulfilled, the problem is vastly more difficult since the electron-ion interaction includes the possibility of bound states. For a hydrogen plasma, the above

result is probably useful for temperatures above about 13 eV, and may give a good estimate for the free energy for a system of known composition for temperatures down to about 7 eV.

RESULTS

The particle densities used in the present calculation – as calculated by the ion-sphere model – are included in Tables III-1 and III-2.

Table III-1
FREE-ELECTRON CONCENTRATION, ρ_e

kT	Air: ρ_e (electrons cm^{-3})						
	J = 1	J = 2	J = 3	J = 4	J = 5	J = 6	
1	1.05 ¹⁷	3.27 ¹⁶	9.67 ¹⁵	2.47 ¹⁵	4.44 ¹⁴	5.25 ¹³	
2	5.75 ¹⁹	2.74 ¹⁸	3.28 ¹⁷	4.23 ¹⁶	5.44 ¹⁵	7.24 ¹⁴	
5	3.32 ²⁰	1.12 ¹⁹	1.33 ¹⁸	1.67 ¹⁷	2.17 ¹⁶	2.87 ¹⁵	
10	1.02 ²¹	3.22 ¹⁹	3.78 ¹⁸	4.72 ¹⁷	6.11 ¹⁶	8.08 ¹⁵	
15	1.88 ²¹	5.82 ¹⁹	6.82 ¹⁸	8.55 ¹⁷	1.11 ¹⁷	1.48 ¹⁶	
20	2.79 ²¹	8.70 ¹⁹	1.03 ¹⁹	1.30 ¹⁸	1.70 ¹⁷	2.27 ¹⁶	

Table III-2
PARTICLE CONCENTRATIONS, N_V

kT	Nitrogen: N_V (nuclei cm^{-3})					
	J = 1	J = 2	J = 3	J = 4	J = 5	J = 6
1	5.25 ¹⁸	5.36 ¹⁷	5.37 ¹⁶	5.38 ¹⁵	5.38 ¹⁴	5.38 ¹³
2	2.34 ²⁰	3.16 ¹⁸	3.32 ¹⁷	3.85 ¹⁶	3.90 ¹⁵	3.97 ¹⁴
5	2.56 ²⁰	5.50 ¹⁸	5.24 ¹⁷	5.64 ¹⁶	6.49 ¹⁵	7.50 ¹⁴
10	4.11 ²⁰	8.81 ¹⁸	8.71 ¹⁷	9.79 ¹⁶	1.23 ¹⁶	1.62 ¹⁵
15	5.53 ²⁰	1.27 ¹⁹	1.39 ¹⁸	1.72 ¹⁷	2.23 ¹⁶	2.96 ¹⁵
20	7.07 ²⁰	1.79 ¹⁹	2.08 ¹⁸	2.62 ¹⁷	3.42 ¹⁶	4.55 ¹⁵
kT	Oxygen: N_V (nuclei cm^{-3})					
	J = 1	J = 2	J = 3	J = 4	J = 5	J = 6
1	5.38 ¹⁸	5.39 ¹⁷	5.37 ¹⁶	5.38 ¹⁵	5.38 ¹⁴	5.38 ¹³
2	3.32 ²⁰	3.77 ¹⁸	3.85 ¹⁷	4.68 ¹⁶	5.58 ¹⁵	5.59 ¹⁴
5	3.02 ²⁰	6.57 ¹⁸	6.45 ¹⁷	6.76 ¹⁶	7.97 ¹⁵	9.25 ¹⁴
10	4.76 ²⁰	1.04 ¹⁹	1.03 ¹⁸	1.12 ¹⁷	1.29 ¹⁶	1.58 ¹⁵
15	6.40 ²⁰	1.42 ¹⁹	1.44 ¹⁸	1.68 ¹⁷	2.14 ¹⁶	2.83 ¹⁵
20	8.01 ²⁰	1.86 ¹⁹	2.04 ¹⁸	2.52 ¹⁷	3.27 ¹⁶	4.34 ¹⁵

Section IV
LINE TRANSITIONS

The absorption coefficient $\mu(\epsilon)$ contains contributions from all transitions, discrete and continuous, which can absorb a photon of frequency ϵ . For a line transition from an atomic state i to a state j the contribution to the absorption coefficient is expressible in terms of the oscillator strength (f-number) f_{ij} as

$$\mu_{i \rightarrow j}(\epsilon) = \frac{\pi e^2}{mc} N_i f_{ij} [2 \pi \hbar b_{ij}(\epsilon)] = 1.0975 \times 10^{-16} N_i f_{ij} b_{ij}(\epsilon) \text{ cm}^{-1} \quad (4.1)$$

where N_i is the population of the initial (lower) state (in number of atoms cm^{-3}) and $b_{ij}(\epsilon)$ represents the shape of the line ($i \rightarrow j$), normalized according to

$$\int_0^\infty b_{ij}(\epsilon) d\epsilon = 1. \quad (\epsilon \text{ in eV}) \quad (4.2)$$

The f-number is a convenient way of expressing the matrix element in a quantum mechanical calculation of the radiative transition probability in the electric-dipole approximation. The definition of the f-number for a transition from an atomic state i with energy E_i to a state j , energy E_j , applicable in L-S coupling, is

$$f_{ij} = \frac{8\pi^2 m}{3h^2} \left(h\nu_{ij} \right) \frac{S_{ij}}{G_i} \quad (4.3)$$

The statistical weight of the lower state, G_i , is $(2S + 1)(2L + 1)$ for a state of total spin S and total orbital angular momentum L . In our units

$$f_{ij} = \frac{1}{3} (E_j - E_i) \frac{S_{ij}}{G_i} \quad (E_j - E_i \text{ in Ry}) \quad (4.4)$$

The "line strength" S_{ij} is given by (Ref. 83)

$$S_{ij} = \mathcal{S}(M)\mathcal{S}(L)\sigma_{ij}^2 \quad (4.5)$$

The factors $\mathcal{S}(L)$ and $\mathcal{S}(M)$ are usually called relative line strengths and relative multiplet strengths. They arise from the angular integration of the matrix element subject to a specific coupling of the angular momenta. In the present calculation J -splitting is consistently ignored so the strengths are summed over all the lines in a multiplet (J is the total angular momentum, orbital plus spin). Since

$$\sum_{JJ'} \mathcal{S}(L) = 1$$

(Ref. 83, p. 443), we require only the factors $\mathcal{S}(M)$. These can be computed from the theory of Ref. 83 and many are tabulated (Ref. 84). The expressions used for $\mathcal{S}(M)$ – considering our summation-over-state conventions – are described in the first subsection below and Table IV-1.

The factor σ_{ij} is the dipole integral (in atomic units)

$$\sigma_{ij} = \frac{1}{\sqrt{(4\ell^2 - 1)}} \int_0^\infty P_i(r) r P_j(r) dr \quad (4.6)$$

where P_i and P_j are r times the radial wave functions of the active electron, and ℓ_{ij} is the greater of the two orbital angular momentum values of the active electron in states i and j . The integration over the coordinates of the passive electrons has been ignored as this is generally close to unity. The dipole integrals employed are Hartree-Fock-Slater (HFS) values (Ref. 85) for transitions between two states each with principal quantum number less than nine. Hydrogenic values are used for transitions between states of higher excitation.

A detailed discussion of the f-number evaluation is in the first subsection; the treatment of line broadening is described in the second subsection. A brief summary of the computer program utilized in the evaluation of the line-transition contribution to the absorption coefficient concludes Sec. IV.

f-NUMBER EVALUATION

The detailed expressions used in the evaluation of f-numbers — the angular factors $\mathcal{S}(M)$, the statistical weights G_{ij} , and the approximations to the radial integrals — depend on the conventions noted in Sec. II regarding summation of the occupation numbers over nearly-degenerate states. Thus, each type of transition is best treated separately.

Consider an initial state ($i^{\alpha}n^{\beta}S^{\gamma}L^{\delta}$) and a final state ($i'^{\alpha'}n'^{\beta'}S'^{\gamma'}L'^{\delta'}$) arranged so that $n' \geq n$. (This notation was defined at the end of Sec. II). The total spin of the initial (final) core is $S_{12}(S'_{12})$ and the total orbital angular momentum of the core is $L_{12}(L'_{12})$. In the one-electron electric-dipole approximation made here, selection rules restrict the possible transitions to final states satisfying the following conditions:

- $i' = i$, since no change of species or degree of ionization is allowed
- $S' = S$, for electric multipole transitions
- $L' = L - 1, L, L + 1$ only, for dipole transitions
- The orbital angular momentum of the electron making the transition must change by one unit

For all allowed transitions considered, the expressions for the angular factors \mathcal{S} (M), the statistical weights G, and the radial integrals may be found among the following cases. The values of Z_k and g_i are listed in Table IV-1.

Table IV-1
ANGULAR FACTORS

Statistical weights

$$g_1 = (2L + 1)(2S + 1)$$

$$g_2 = (2S + 1)(2L_{12} + 1)(2\ell + 1)$$

$$g_3 = 2(2\ell + 1)(2S_{12} + 1)(2L_{12} + 1)$$

$$g_4 = 2(n^2 - 16)(2S_{12} + 1)(2L_{12} + 1)$$

$$g_5 = 2n^2(2S_{12} + 1)(2L_{12} + 1)$$

Angular parameter

n_s (n'_s)—number of 2s-electrons in initial (final) state

n_p (n'_p)—number of 2p-electrons in initial (final) state

S_1 (S'_1)—total spin of 2s-electrons in initial (final) state

S_2 (S'_2)—total spin of 2p-electrons in initial (final) state

L_1 (L'_1)—total orbital angular momentum of 2s-electrons in initial (final) state

L_2 (L'_2)—total orbital angular momentum of 2p-electrons in initial (final) state

$F(q, S, L; S', L') = |(p^q S L \{ |p^{q-1} (S' L') p S L\})|^2$ is the square of the fractional parentage coefficient (Ref. 86).

$U(\dots)$ is the U-coefficient of Jahn as defined in Ref. 87.

$$Z_1 = n_s(n_p + 1) F(n'_p, S'_2, L'_2; S'_2, L'_2) (2L'_{12} + 1)(2S_{12} + 1) U^2\left(\frac{1}{2}, S'_1, S_2, S; S_1, S'_2\right)$$

$$Z_2 = n_s(2L' + 1)(2S + 1) U^2\left(\frac{1}{2}, S'_1, S, S_2; S_1, S'_{12}\right)$$

Table IV-1 (cont'd)

$$Z_3 = n_p F(n_p, S'_2, L'_2; S_2, L_2) (2L+1) (2S+1) U^2 \left(\frac{1}{2}, S'_2, S, S_1; S_2, S'_{12} \right)$$

$$Z_4 = 10 n_p F(n_p, S'_2, L'_2, S_2, L_2) (2L+1) (2S+1) U^2 \left(\frac{1}{2}, S'_2, S, S_1; S_2, S'_{12} \right)$$

$$\times U^2(L, 1, L'_2, 2; L', 1)$$

$$Z_5 = 10 Z_3$$

$$Z_6 = 3 n_s (2L+1) (2S+1) U^2 \left(\frac{1}{2}, S'_1, S, S_2; S_1, S'_{12} \right)$$

$$Z_7 = (2L'+1) (2S+1)$$

$$Z_8 = 6 (2L+1) (2S+1) U^2 (L, 1, L_2, 1; L', 2)$$

$$Z_9 = (2L+1) (2S+1)$$

$$Z_{10} = 10 (2L+1) (2S+1) U^2 (L, 1, L_2, 2; L', 1)$$

$$Z_{11} = n_s (n_p + 1) (2L'+1) (2S+1) U^2 (L_2, l, 1, L'; L, L'_2) F(n'_p, S_2, L_2, S'_2, L'_2).$$

$$U^2 \left(\frac{1}{2}, S'_1, S_2, S_{12}; S_1, S'_2 \right)$$

$$Z_{12} = n_s (n_p + 1) (2L'_2 + 1) \frac{(2L+1) (2S+1)}{(2L_2 + 1)} U^2 \left(\frac{1}{2}, S'_1, S_2, S_{12}; S_1, S'_2 \right).$$

$$F(n'_p, S_2, L_2, S'_2, L'_2)$$

$$Z_{13} = n_s (n_p + 1) (2L'+1) (2S+1) U^2 \left(\frac{1}{2}, S'_1, S_2, S_{12}; S_1, S'_2 \right).$$

$$F(n'_p, S_2, L_2, S'_2, L'_2)$$

$$Z_{14} = 5 n_s (n_p + 1) (2L'_2 + 1) (2S+1) U^2 \left(\frac{1}{2}, S'_1, S_2, S_{12}; S_1, S'_2 \right).$$

$$F(n'_p, S_2, L_2; S'_2, L'_2)$$

Table IV-1 (cont'd)

$$Z_{15} = 30(2L_2 + 1)(2S + 1)$$

$$Z_{16} = 105(2L_2 + 1)(2S + 1)$$

$$Z_{17} = 2n_s(n_p + 1)(2L'_2 + 1)(2S_{12} + 1)n^2 F(n'_p, S_2, L_2, S'_2, L'_2).$$

$$U^2\left(\frac{1}{2}, S'_1, S_2, S_{12}; S_1, S'_2\right)$$

$$Z_{18} = 2n_s(n_p + 1)(2L'_2 + 1)(2S_{12} + 1)F(n'_p, S_2, L_2, S'_2, L'_2).$$

$$U^2\left(\frac{1}{2}, S'_1, S_2, S_{12}; S_1, S'_2\right)(2\ell + 1)$$

$$Z_{19} = [(n^2 - 16)/n^2]Z_{17}$$

$$Z_{20} = 2\ell(4\ell^2 - 1)(2L_{12} + 1)(2S_{12} + 1)$$

$$Z_{21} = 2\ell'(4\ell'^2 - 1)(2L_{12} + 1)(2S_{12} + 1)$$

$$Z_{22} = n_p(2L + 1)(2S + 1)U^2\left(\frac{1}{2}, S'_2, S, S_1; S_2, S'_{12}\right)$$

n = 2. Initial state split into L-S components. Final states with $n' \geq 9$ are rejected as such lines are quite weak. HFS values of σ^2 are used.

$n' = 2$	$(2s \rightarrow 2p)$	$\mathcal{S}(M) = Z_1$	$G = g_1$
$n' = 2$	$(2s \rightarrow 3p)$	$= Z_2$	$= g_1$
	$(2p \rightarrow 3s)$	$= Z_3$	$= g_1$
	$(2p \rightarrow 3d)$	$= Z_4$	$= g_1$
	$L' \neq 9$	$= Z_5$	$= g_1$
$n' = 4-9$	$(2s \rightarrow n'p)$	$= Z_6$	$= g_1$
	$(2p \rightarrow n's)$	$= Z_{22}$	$= g_1$
	$(2p \rightarrow n'd)$	$= Z_5$	$= g_1$

$n = 3$. Initial state split into L-S components unless $L = 9$, in which case the occupation numbers are summed over L for the given S. Final states with $n' \geq 9$ are rejected. HFS values of σ^2 are used. If $L \neq 9$, $G = g_1$; if $L = 9$, $G = g_2$.

$n' = 3$	$\gamma \neq \gamma'$	$(2s \rightarrow 2p)$	$L \neq 9, L' \neq 9$	$\mathcal{S}(M) = Z_{11}$	$G = g_1$
			$L \neq 9, L' = 9$	$= Z_{12}$	$= g_1$
			$L = 9, L' \neq 9$	$= Z_{13}$	$= g_2$
			$L = 9, L' = 9$	$= Z_{14}$	$= g_2$
$\gamma = \gamma'$		$(3s \rightarrow 3p)$		$= Z_7$	$= g_1 \text{ or } g_2$
		$(3d \rightarrow 3p)$	$L = 9$	$= 10 Z_7$	$= g_2$
			$L \neq 9$	$= Z_8$	$= g_1$
		$(3p \rightarrow 3s)$		$= Z_9$	$= g_1 \text{ or } g_2$
		$(3p \rightarrow 3d)$	$L' = 9$	$= 10 Z_9$	$= g_1 \text{ or } g_2$
			$L' \neq 9$	$= Z_{10}$	$= g_1 \text{ or } g_2$
$n' = 4-9$		$(3s \rightarrow n'p)$		$= 3 Z_9$	$= g_1 \text{ or } g_2$
		$(3p \rightarrow n's)$		$= Z_9$	$= g_1 \text{ or } g_2$
		$(3p \rightarrow n'd)$		$= 10 Z_9$	$= g_1 \text{ or } g_2$
		$(3d \rightarrow n'p)$	$L = 9$	$= Z_{15}$	$= g_2$
			$L \neq 9$	$= 6 Z_9$	$= g_1$
		$(3d \rightarrow n'f)$	$L = 9$	$= Z_{16}$	$= g_2$
			$L \neq 9$	$= 21 Z_9$	$= g_1$

$n = 4-8$. Occupation numbers of initial states summed over all L-S components. Final states with $n' > 16$ are rejected.

$\gamma \neq \gamma'$ require $n = n'$, $\ell = \ell'(2s - 2p)$

$\ell < 4$: $\mathcal{S}(M) = Z_{18}$, $G = g_3$, HFS σ^2 with outer (n, ℓ) electron

$\ell = 4$: $\mathcal{S}(M) = Z_{19}$, $G = g_4$, HFS σ^2 with outer $(n, \ell = 3)$ electron

$\gamma = \gamma'$ $n' < 9$: $\ell \neq 1, \ell' = \ell - 1$: $\mathcal{S}(M) = Z_{20}$, $G = g_3$, HFS σ^2

$\ell' = \ell + 1$: $\mathcal{S}(M) = Z_{21}$, $G = g_3$

$\ell < 3$: HFS σ^2

$\ell = 3$: hydrogenic f-number

$\ell = \ell' = 4$: Sum of hydrogenic f-numbers over

$\ell' = \ell \pm 1$ averaged over $\ell = 4$

to $(n - 1)$ according to

$$\frac{1}{(n^2 - 16)} \sum_{\ell=4}^{(n-1)} (2\ell + 1) [f_{n\ell}^{n', \ell-1} + f_{n\ell}^{n', \ell+1}]$$

$n' = 9-16$, $\ell \neq 4$: Sum of hydrogenic f-numbers over

$\ell' = \ell \pm 1$

$\ell = \ell' = 4$: Same average as for $n' < 9$

$n = 9-16$. Occupation numbers of initial states summed over all L-S components and over all angular momentum states ℓ . Final states with $n' > 16$ are rejected.

$\gamma \neq \gamma'$ require $n = n', \ell = \ell'(2s - 2p)$

$\mathcal{S}(M) = Z_{17}$, $G = g_5$, HFS σ^2 with outer (8f) electron

$\gamma = \gamma'$ shell-averaged f-numbers from Ref. 88. Initial states $n > 16$ not considered. The hydrogenic f-numbers are from the tables in Ref. 89.

LINE BROADENING

A comprehensive review of the theory of line broadening in a plasma has recently been published (Ref. 90). Stewart and Pyatt (Ref. 8) discuss approximations to this theory relevant to high-temperature opacity studies, and the present calculation follows their treatment quite closely.

As a result of the interaction of the radiating atom with the plasma each line is assumed to acquire a Lorentz shape

$$b_{ij}^{(L)}(\epsilon) = \frac{w_j/\pi}{(E - E_j + E_i)^2 + w_j^2} \quad (4.7)$$

with a width w_j proportional to the electron density ρ_e . Following Stewart and Pyatt (Ref. 8) only the upper state j is assumed to be perturbed, and asymmetric corrections to Eq. (4.7) due to overlapping lines and effects due to ion perturbers have been ignored. With these approximations an expression for the width is given by Baranger [Ref. 90, Eq. (113)]

$$w_j = \int_0^\infty f(v) dv \frac{4\pi}{3} \rho_e v \left(\frac{\hbar}{mv}\right)^2 \sum_k \left\{ \frac{\text{Max}(\ell_j, \ell_k)}{(2\ell_j + 1)} \left[\int_0^\infty p_j(r) p_k(r) dr \right]^2 \frac{\pi}{\sqrt{3}} g(j, k) \right\} \quad (4.8)$$

in terms of an average over a Maxwellian distribution $f(v)$ in electron velocity v of the same radial matrix elements σ_{jk}^2 as determine the line strengths [Eq. (4.6)] multiplied by a bremsstrahlung Gaunt factor $g(j, k) \geq 1$. The Gaunt factor is usually close to unity, so, following Stewart and Pyatt, we set $g(j, k) = 1$ and evaluate the sum over σ_{jk}^2 by a sum rule (Refs. 91 and 92).

$$\sum_k \frac{\text{Max}(\ell_j, \ell_k)}{(2\ell_j + 1)} \left[\int_0^\infty p_j(r) r p_k(r) dr \right]^2 = \frac{1}{2} \left(\frac{v_1}{Z_{\text{RES}}} \right)^2 \left[5v_j^2 + 1 - 3\ell_j(\ell_j + 1) \right] \quad (4.9)$$

Z_{RES} is the charge of the passive ion (one greater than the initial charge of the system) and ν_j is the effective quantum number (Ref. 92) of the state j

$$\left(\frac{\nu_j}{Z_{RES}}\right)^2 = 1/[E_I(j) - E_j] \quad (\text{Ry}) \quad (4.10)$$

where $E_I(j)$ is the ionization energy of the active electron in the passive ion. The Maxwell average of $1/v$ is $(2m/\pi kT)^{1/2}$. The result used for the width is

$$w_j = (0.637 \times 10^{-22}) \frac{\rho_e (\text{cm}^{-3})}{\sqrt{kT(\text{eV})}} \left(\frac{\nu_j}{Z_{RES}}\right)^2 \left[5\nu_j^2 + 1 - 3\ell_j(\ell_j + 1) \right] (\text{eV}) \quad (4.11)$$

By averaging this expression over ℓ_j and replacing the effective quantum number ν_j by the principal quantum number n_j , the result obtained corresponds to Eq. (31) of Ref. 8.

The mechanism of line broadening in this approximation is inelastic scattering of a free electron by the radiating atom - a real, energy-conserving transition. Thus, the summation over states k in Eq. (4.8) must be restricted to states energetically accessible to the radiating atom in collisions with electrons of velocity v , before averaging over velocity. The use of the sum rule ignores this restriction and so overestimates the width. Setting the Gaunt factor to unity underestimates the width, so the two approximations taken together should be better than either alone.

Since the width increases as the fourth power of the principal quantum number the assumption of broadening in the upper state only should be valid except for same-shell transitions. However, following Stewart and Pyatt, the present calculation has used Eq. (4.11) for all transitions except those $2s-2p$ transitions for which $\nu_j < 1$. Here the s-state broadening is assumed to dominate so $\ell_j = 0$ in Eq. (4.11).

At the high temperatures considered, Doppler broadening may become a significant line-broadening mechanism — particularly near line centers. To include this effect properly in the line shape, the Lorentz profile $b^L(\epsilon)$, Eq. (4.7), is folded with a Doppler function (Ref. 90) and the resulting distribution is

$$b^{(D)}(\epsilon) = \frac{2}{\sqrt{\pi} \delta} \int_{-\infty}^{\infty} d\epsilon' b^L(\epsilon') \exp \left[- \left(\frac{\epsilon - \epsilon'}{\delta/2} \right)^2 \right], \quad \delta = 2 \left(\frac{2kT}{Mc^2} \right)^{1/2} \epsilon_c \quad (4.12)$$

for radiating atoms of mass M and lines centered at ϵ_c . This result may be expressed in terms of the probability integral for complex argument and is tabulated in Ref. 93 where useful series expansions are also given. For $w > 5\delta$ or $(\epsilon - \epsilon_c) > 5\delta$, $b^{(D)}(\epsilon)$ approaches very closely a Lorentz function.

For highly-excited states the line width of Eq. (4.1) will approach the energy interval between adjacent states of the isolated system. Such states appear as a quasi-continuum and are said to be merged. A treatment of this problem according to the electron-impact theory of Baranger has recently been published (Ref. 94) and the result is

$$n_m^7 / Z_{RES}^4 = 0.4107 \left[\frac{10^{23}}{\rho_e (\text{cm}^{-3})} \right] \sqrt{kT(\text{eV})} \quad (4.13)$$

n_m is the critical quantum number in the sense that electron states with principal quantum number greater than n_m are merged into the continuum. This result has been used in the present calculation, transitions from states below n_m to states above are included in the photoionization calculation, and the photoionization edge is lowered accordingly. Thus n_m serves as a cutoff for high n -values. For transitions between two states both lying above n_m , the contribution should be included among the free-free transitions. However, this was not done in the present calculation. This contribution was neglected as unwarranted in view of the low accuracy (hydrogenic approximation) of the free-free cross sections employed. In order to include it, the free-free electron concentration should be increased by the concentration of electrons in the bound states having $n > n_m$.

The values of n_m calculated by Eq. (4.13) for the temperatures and densities of the present work are listed in Table IV-2.* Equation (4.13) is derived assuming $n_m \gg 1$, so the small n_m values in Table IV-2 are suspect. Further, so large an extrapolation of our approximation to the photoionization cross section below its vacuum edge is certainly less reliable than the HFS f-number calculations even though the resulting lines are broadened into a quasi-continuum. Therefore, the present calculation evaluates n_m for Eq. (4.13) and chooses as the critical quantum number the larger of the so-calculated n_m and 7.

Table IV-2
LINE MERGING LIMITS EVALUATED FROM EQ. (4.13)

kT (eV)	Merging Limit					
	J ^(a) = 1	J = 2	J = 3	J = 4	J = 5	J = 6
1	6.3	7.4	8.8	10.7	13.7	18.6
2	3.7	5.8	7.8	10.5	14.0	18.7
5	3.1	5.0	6.8	9.2	12.3	16.4
10	2.8	4.6	6.2	8.3	11.1	14.9
15	2.6	4.3	5.9	7.9	10.5	14.0
20	1.8	3.0	4.0	5.4	7.3	10.0

(a) J is defined in the table of densities at the conclusion of Sec. III.

COMPUTER CODE MULTIPLET

To provide a table of the frequencies, strengths, and widths of all the radiative bound-bound atomic transitions relevant to a given temperature and density of oxygen or nitrogen, and to provide a frequency-dependent absorption coefficient due to such transitions over an arbitrary energy grid a computer program, MULTIPLET, has been devised. The program is coded in the FORTRAN II (Version III) language and has been operated on an IBM-7094 computing system.

*In computing these values of n_m , Z_{RES} in Eq. (4.13) was inadvertently set equal to 1. Hence, these entries are actually $n_m/Z_{RES}^{4/7}$ rather than n_m . The effect of this error on the final results should be small since the lower limit of $n_m = 7$ was used rather than n_m itself when $n_m < 7$.

The initial data upon which the calculation operates are cards which specify the state of the gas at a given temperature and six values of the density. For each atomic state as described in Sec. II, there is one card containing the identification (iyn&SL), the energy of the state (in eV relative to the ground state of the neutral atom of the species), and six occupation numbers α_j ($J = 1 - 6$) provided by the statistical mechanical calculation described in Sec. III. The occupation numbers are normalized such that the sum of α_j over all the cards in a set is unity for a given temperature, species, and for each density J .

Bound-bound transitions can take place only between atomic states represented by such cards. Thus, the number of states, both initial and final, to be considered for the gas at the given temperature and densities is determined by the number of cards in the data deck. The data decks used in the present calculation contain all states with occupation numbers $\alpha_j \geq 10^{-8}$. In addition some cards with zero occupation have been included to serve as possible final states, although the completeness of such states is not certain. However, an attempt has been made to include all such relevant states.

The program, MULTIPLET, is conveniently broken down into three phases: in the first, all the cards of the data deck are read and listed, all pairs of states are compared by application of the appropriate selection rules, and for each allowed transition the line frequency and the angular factor (Table 4-1) are evaluated. In this procedure only those initial states are considered one of whose occupation numbers is greater than an arbitrary cutoff α_0 — set equal to 10^{-3} in the present calculation. The resulting transitions are arranged in order of increasing line frequency, and the frequency, angular factor, and initial and final state data are written onto magnetic tape.

The second phase reads the transition data of Phase 1 from tape, one transition at a time, evaluates the f-number and collision and Doppler widths as described above, and writes this information on another tape — the line atlas. The line atlas contains data completely describing each transition: the line frequency, f-number, radial integral σ^2 of Eq. (4.6), the collision and Doppler widths, the energy and identification of both the initial and final atomic states, and the occupation numbers of the initial states.

The line atlas is listed by the program and serves as the source datum for any desired frequency averages of the absorption coefficient.

The final phase of MULTIPLET is concerned with generating from the data in the line atlas a frequency-dependent absorption coefficient $\mu(\epsilon)$ over an arbitrary set of energies ϵ_N :

$$\mu(\epsilon) = \sum_{i < j} \mu_{ij}(\epsilon) \quad \text{cm}^{-1} \quad (4.14)$$

where $\mu_{ij}(\epsilon)$ is defined in Eq. (4.1). For each desired set of equally-spaced energies the program is provided with a data card containing $(N_\omega, \omega_0, \Delta\omega)$, where N_ω (≤ 2000) is the number of energies at which the absorption coefficient is to be tabulated and $\epsilon_N = \omega_0 + (N-1)\Delta\omega$, ($N = 1 \rightarrow N_\omega$), specifies the energy set.

The occurrence of very small line widths ($\sim 10^{-4}$ eV) at low densities makes it impractical to choose $\Delta\omega$ sufficiently small to adequately represent such narrow lines. Thus, for calculational purposes, lines are classed as broad lines (width $w \geq \frac{1}{2} \Delta\omega$) and narrow lines ($w < \frac{1}{2} \Delta\omega$). The line centers of broad lines are shifted to the nearest energy ϵ_N and the line shape is included in the table of the absorption coefficient. Narrow lines must be treated separately depending on the type of frequency average desired. Two such averages are described in Sec. VI — the Planck mean and the Rosseland mean opacity.

A complete FORTRAN listing of MULTIPLET is included in Appendix B.

Section V

PHOTOIONIZATION TRANSITIONS

The contribution to the absorption coefficient of photoionization transitions from an atomic state i is conveniently expressed in terms of the total photoionization cross section $\sigma_i(\epsilon)$ (cm 2) as

$$\mu(\epsilon) = \sum_i N_i \sigma_i(\epsilon) \quad \text{cm}^{-1} \quad (5.1)$$

where N_i is the population of the state i (in number of atoms cm $^{-3}$).

Each atomic state will, in general, give rise to several different photoionization transitions, corresponding to different states of the residual atom, and for each there is a separate cross section $\sigma_{ij}(\epsilon)$ and energy threshold ϵ_{ij}^T . Thus

$$\sigma_i(\epsilon) = \sum_j \sigma_{ij}(\epsilon)$$

summed over all states j for which $\epsilon_{ij}^T \leq \epsilon$.

As described in Sec. II the general initial state ($i\gamma nISL$) treated in the present calculation may be written

$$2s^{n_s} 2p^{n_p} \left(\begin{smallmatrix} S_{12} \\ L_{12} \end{smallmatrix} \right) nL(S_L)$$

with the K-shell $1s^2$ understood and the configuration

$$2s^{n_s} 2p^{n_p} \left(\begin{smallmatrix} S_{12} \\ L_{12} \end{smallmatrix} \right)$$

specified by the core index γ (Table II-1). A general photoionization transition from such an initial state may be written

$$2s^{n_s} 2p^{n_p} \left(S_{12} L_{12} \right) n\ell \left(S_L \right) \rightarrow 2s^{n'_s} 2p^{n'_p} \left(S_c L_c \right) n'\ell' \left(S'' L'' \right) \epsilon \ell'' \left(S' L' \right) \quad (5.2)$$

where the final state consists of a free electron with energy ϵ and orbital angular momentum ℓ'' and a residual atom

$$2s^{n'_s} 2p^{n'_p} \left(S_c L_c \right) n'\ell' \left(S'' L'' \right).$$

In the one-electron, electric-dipole approximation considered here the possible final states are limited by selection rules:

- (a) $S' = S$, for electric multipole transitions in LC coupling
- (b) $L' = L - 1, L, L + 1$ only, for dipole transitions.
- (c) $\ell'' = \ell_0 \pm 1 \geq 0$, where ℓ_0 is the initial orbital angular momentum of the electron being ejected.

For the photoionization from a multiply-occupied initial state, a parentage expansion (Ref. 95) will give rise in general to several possible states of the residual atom — each with a different energy threshold ϵ^T and coefficient of fractional parentage F_p . An enumeration of the possibilities follows:

- (a) Ejection of an outer (n, ℓ) electron

$$2s^{n_s} 2p^{n_p} \left(S_{12} L_{12} \right) n\ell \left(S_L \right) \rightarrow 2s^{n_s} 2p^{n_p} \left(S_{12} L_{12} \right) \epsilon \ell' \left(S_{L'} \right)$$

Here $n'_s = n_s$, $n'_p = n_p$, $S_c = S'' = S_{12}$, $L_c = L'' = L_{12}$, $\ell' = \ell \pm 1 \geq 0$.

(b) Ejection of a 2p outer electron: Decomposing the initial state into parents;

$$2s^{n_s} 2p^{n_p}(S_L) = \sum_p F_p \left[2s^{n_s} 2p^{n_p-1} \left(\begin{smallmatrix} S_p \\ L_p \end{smallmatrix} \right) 2p(S_L) \right],$$

every pair of values $\left(\begin{smallmatrix} S_p \\ L_p \end{smallmatrix} \right)$ for which

$$F_p = \left| \left(\begin{smallmatrix} n_p \\ p \end{smallmatrix} \right) \left(\begin{smallmatrix} n_p-1 \\ p \end{smallmatrix} \right) \left(\begin{smallmatrix} S_p \\ L_p \end{smallmatrix} \right) pSL \right|^2$$

is nonvanishing constitutes a possible final state of the residual atom with

$$n'_s = n_s, \quad n'_p = n_p - 1, \quad S_c = S_p, \quad L_c = L_p \quad \text{and} \quad \ell' = 0 \text{ or } 2.$$

(c) Ejection of a 2s outer electron: Decomposing the initial state into parents,

$$2s^{n_s}(S_L) = \sum_p F_p \left[2s^{n_s-1} \left(\begin{smallmatrix} S_p \\ L_p \end{smallmatrix} \right) 2s(S_L) \right]$$

the only possible states are

$$n_s = 2: \quad S = 0, \quad L = 0; \quad S_p = \frac{1}{2}, \quad L_p = L = 0, \quad F_p = 2$$

or

$$n_s = 1: \quad S = \frac{1}{2}, \quad L = 0; \quad S_p = 0, \quad L_p = L = 0, \quad F_p = 1,$$

in both of which

$$n'_s = n_s - 1, \quad S_c = S_p, \quad L_c = L_p, \quad \ell' = 1.$$

(d) Ejection of a 2p inner electron. Decoupling one 2p electron from the rest

$$2s^{n_s} 2p^{n_p} \left(\begin{smallmatrix} S_{12} \\ L_{12} \end{smallmatrix} \right) n\ell(S_L) = \sum_p F'_p \left[2s^{n_s} 2p^{n_p-1} \left(\begin{smallmatrix} S_{pL_p} \\ L_p \end{smallmatrix} \right) 2p \left(\begin{smallmatrix} S_{12} \\ L_{12} \end{smallmatrix} \right) n\ell(S_L) \right]$$

$$F'_p = \left| \left(\begin{smallmatrix} n_p \\ p \end{smallmatrix} S_{12} L_{12} \left| \begin{smallmatrix} n_p-1 \\ p \end{smallmatrix} (S_{pL_p}) p S_{12} L_{12} \right. \right) \right|^2$$

the outer (n, ℓ) electron must be coupled to $\left(\begin{smallmatrix} S_{pL_p} \\ L_p \end{smallmatrix} \right)$, so the recoupled initial state may be written

$$\sum_{pS'L''} F_p(S''L'') \left[2s^{n_s} 2p^{n_p-1} \left(\begin{smallmatrix} S_{pL_p} \\ L_p \end{smallmatrix} \right) n\ell(S''L'') \right] 2p(S_L)$$

where $F_p = F'_p U^2 \left(\begin{smallmatrix} \ell \\ L_p \end{smallmatrix} L_1 ; L'' L_{12} \right) U^2 \left(\frac{1}{2} S_p S \frac{1}{2} ; S'' S_{12} \right)$ and the U-functions are the Jahn coefficients of Ref. 87. Experimentally the energies of states with different values of $(S''L'')$ usually vary much less than do the energies of states with different $\left(\begin{smallmatrix} S_{pL_p} \\ L_p \end{smallmatrix} \right)$. Therefore the $(S''L'')$ -splitting of the photoionization edges is ignored and the sum over $(S''L'')$ is carried out directly, leading to final states $2s^{n'_s} 2p^{n'_p-1} \left(\begin{smallmatrix} S_{pL_p} \\ L_p \end{smallmatrix} \right) n\ell$ with probability F'_p . So $n'_s = n_s$, $n'_p = n_p - 1$, $S_c = S_p$, $L_c = L_p$, $\ell' = 0, 2$.

(e) Ejection of a 2s inner electron. Decomposing the initial state as in Case (d)

$$2s^{n_s} 2p^{n_p} \left(\begin{smallmatrix} S_{12} \\ L_{12} \end{smallmatrix} \right) n\ell(S_L) = \sum_{pS'} F_p(S'') \left[2s^{n_s-1} 2p^{n_p} \left(\begin{smallmatrix} S_{pL_{12}} \\ L_{12} \end{smallmatrix} \right) n\ell(S''L) \right] 2s(S_L)$$

$$F_p(S'') = F'_p U^2 \left(\frac{1}{2} S_p S \frac{1}{2} ; S'' S_{12} \right), \quad F'_p = \left(\frac{2S_p + 1}{2S + 1} \right).$$

As in Case (d), the sum over S' is carried out directly, leading to final states $2s^{n_s-1} 2p^{n_p} (S_p L_{12}) n'_p(L)$ with probability F'_p . So $n'_s = n_s - 1$, $n'_p = n_p$, $S_c = S_p$, $L_c = L_{12}$, and $\ell' = 1$.

Such a decomposition of the initial state into substates each with a different ionization potential results in a splitting of the photoionization edges. For calculations of Planck mean opacities at high temperatures (Sec. VI) this splitting should yield results only slightly different from a calculation in which splitting is ignored. However, the splitting of the 2p-edges is typically a few electron volts in magnitude and so should affect the present low-temperature Planck mean opacities. Rosseland mean opacities should be more sensitive to splitting due to the filling in of regions in the frequency spectrum where the absorption coefficient without splitting would have small values.

Once the initial atomic state i is decomposed into all possible final states of the residual ion, the photoionization cross section σ_{ij} is evaluated in the one-electron, electric-dipole approximation. For a transition from an initial bound electronic state (n, ℓ) to a final state of the free electron with energy ϵ , the photoionization cross section may be written (Ref. 4)

$$\sigma_{ij}(\epsilon) = \frac{16\pi^3 e^2 \omega}{3c} F_p \left[\left(\frac{\ell}{2\ell + 1} \right) (R_{nl}^{\epsilon, \ell-1})^2 + \left(\frac{\ell + 1}{2\ell + 1} \right) (R_{nl}^{\epsilon, \ell+1})^2 \right], \quad (5.3)$$

for photon frequency ω , in terms of the integrals $R_{nl}^{\epsilon \ell'}$ over the radial wave functions

$$R_{nl}^{\epsilon \ell'} = \int_0^\infty r^2 dr R_{\epsilon, \ell'}(r) r R_{nl}(r). \quad (5.4)$$

This result has been derived assuming L-S coupling with the neglect of spin-orbit interaction, and the wave function of the final free electron state, $R_{\epsilon \ell'}(r)$, is normalized on the energy scale

$$\int_0^\infty r^2 dr R_{\epsilon' \ell'}(r) R_{\epsilon \ell'}(r) = \delta(\epsilon' - \epsilon). \quad (5.5)$$

Thus the only unknown quantities in Eq. (5.3) are the radial matrix elements $R_{nl}^{el'}$. In most previous work (Refs. 4, 8, and 9) these matrix elements have been approximated by hydrogenic values.

For electrons with initial-state principal quantum number $n \geq 6$ or orbital angular momentum $l \geq 2$ hydrogenic results have been used here. For smaller values of these quantum numbers, some recently obtained, and significantly more accurate expressions for the radial matrix elements are used. For small values of the electron final energy, the approximation of Burgess and Seaton (Ref. 94) is used and is discussed in the first of the subsequent subsections. An approximation valid for high-energy electrons is described in the second, and the third presents some comparisons with more detailed Hartree-Fock calculations. The final subsection contains a brief summary of the computer program utilized in the evaluation of the photoionization contribution to the absorption coefficient.

THE LOW-ENERGY THEORY

Recently, Burgess and Seaton (Ref. 96) have presented an approximation to the radial matrix elements in terms of the asymptotically correct wave functions. This approximation derives from the observation of Bates and Damgaard (Ref. 92) that the major contribution to the radial integral for bound-bound transitions usually comes from values of r sufficiently large that the effective potential is a Coulomb potential. Replacing the actual one-electron wave function by its asymptotic form — a linear combination of the regular and irregular Coulomb wave functions for the observed value of the energy, modified for small r to ensure convergence of the radial integrals — Bates and Damgaard evaluated the radial matrix elements $R_{nl}^{n'l'}$ and presented their results in tabular form.

Burgess and Seaton (Ref. 96) applied similar considerations to the evaluation of the radial matrix elements $R_{nl}^{el'}$ for bound-free transitions. Whereas the asymptotic behavior of the bound-state wave function is determined by the physically-observed

energy of the bound state, the large-radius behavior of the free-electron wave function, at a given energy, is determined by a phase shift $\delta_{\ell}(L', \epsilon)$. In the approximation of asymptotically correct wave functions, Burgess and Seaton numerically evaluated the radial matrix elements and parameterized the resulting photoionization cross section [Eq. (5.3)] in the form

$$\sigma(\epsilon) = \sigma_0 \sum_{\ell' = \ell \pm 1} C_{\ell\ell'}(L') \frac{G_{\ell\ell'}^2(\nu) \cos^2 [\varphi(\ell, \ell', \nu; \epsilon) + \delta_{\ell}(L', \epsilon)]}{[1 + \epsilon \nu^2]^{2\gamma_{\ell\ell'}(\epsilon)-1}} \quad (5.6)$$

where L' is the orbital angular momentum of the total system in the final state. The quantities $C_{\ell\ell'}(L')$ are the results of the angular integrations and may be simply expressed in terms of Racah coefficients as described in Ref. 96. G , γ , and φ are tabulated by Burgess and Seaton as functions of ν for various combinations of ℓ and ℓ' , and ϵ is the electron kinetic energy in rydbergs divided by Z^2 . The basic variable of the theory, ν , is defined by

$$\nu = Z \left(\frac{1/\lambda_H}{1/\lambda'' - 1/\lambda} \right)^{1/2} \quad (5.7)$$

where

$$1/\lambda_H = 1 \text{ Ry cm}^{-1} = 109,737.3 \text{ cm}^{-1}$$

$$1/\lambda = \text{term value of the initial state (cm}^{-1}\text{)}$$

$$1/\lambda'' = \text{term limit obtained by removing the initial (n, \ell) electron and leaving the residual ion in its final state (cm}^{-1}\text{)}$$

$$Z = \text{charge of the residual ion}$$

The dimensional constant σ_0 of Eq. (5.6) is given in terms of the Bohr radius a_0 by

$$\sigma_0 = \frac{4\pi}{3} \alpha a_0^2 \left(\frac{\nu^2}{Z^2} \right) [\zeta(\nu)]^{-1} = \frac{8.559 \times 10^{-19} \text{ cm}^2}{\zeta(\nu)} \left(\frac{\nu^2}{Z^2} \right) \quad (5.8)$$

where $\xi(\nu)$ is a normalization correction to the asymptotic bound state wave function and may be estimated from knowledge of the physical bound states of the system. For example, the evaluation of $\xi(\nu)$ for the outer electron in the configuration $1s^2 2s^2 2p^2 (S_c L_c) nl (S_L)$ is obtained from consideration of the series obtained by varying n with everything else fixed. The observed energies, $\epsilon_{n'l}$, of the terms in the resulting series, relative to the series ionization limit $I_l = \lim_{n' \rightarrow \infty} \epsilon_{n'l}$, are written

$$(\epsilon_{n'l} - I_l) = -1/\nu_{n'l}^2 \quad (5.9)$$

in terms of their effective quantum number $\nu_{n'l}$, and the quantum defect, $\mu_{n'l}$, is defined by

$$\mu_{n'l} = n' - \nu_{n'l} \quad (5.10)$$

Seaton (Ref. 97) has shown that the so-defined quantum defect μ_{nl} is a continuous, analytic function of the energy (for fixed l) which may be written $\mu_l \left(\frac{-1}{\nu^2} \right)$. Further, $\mu_l \left(\frac{-1}{\nu^2} \right)$ must tend to an integer as ν tends to any one of the integers $0, 1, \dots, l$. Then $\xi(\nu)$ of Eq. (5.8) is given by

$$\xi(\nu) = 1 + \frac{d\mu_l}{d\nu} = 1 + \frac{2}{3} \frac{\partial \mu_l(\epsilon)}{\partial \epsilon} \xrightarrow{\nu \rightarrow \infty} 1 \quad (5.11)$$

evaluated at the observed physical energy ϵ_{nl} of the state (nl) whose normalization is required.

Thus, to estimate $\xi(\nu)$ the observed energy of at least one additional term of the $(n'l)$ series of the initial state (n,l) is required. For outer (n,l) electrons, such states are included in the initial set of energies described in Sec. 2 - at least upon relaxation of the condition that the outer coupling S_L be fixed. For inner

electrons, however, in the presence of an excited outer electron [e.g., the 2p orbital in the state $2s^2 2p^2(^3P)3s$ of NI] the excited state necessary to estimate $\xi(\nu)$ is a doubly-excited state [$2s^2 2p(^2P)3s 3p$ in the preceding example]. The energies of such states are generally not known. The present calculation uses an approximation of Seaton (Ref. 97) for such inner 2p-orbitals

$$\xi(\nu) = \frac{(\nu - 1)(\nu + 2)}{\nu(\nu + 1)}$$

and chooses $\xi = 1.0$ for inner 2s-orbitals. Some comparisons with Hartree-Fock solutions indicate this approximation is reasonable.

For the phase shift $\delta_{\ell}(L', \epsilon)$ of the free-electron final state, Seaton (Ref. 97) has shown that a low-energy approximation is given by extrapolating the quantum defect $\mu_{\ell}(\epsilon)$, Eq. (5.10), of the series containing the final state to small positive energies according to

$$\delta_{\ell}(\epsilon, L') = \pi \mu_{\ell}(\epsilon) \quad (5.12)$$

Moiseiwitsch (Ref. 98) has demonstrated that this result corresponds to an effective-range expansion about the physical bound states.

For electrons with principal quantum number $n > 3$ the initial-state occupation numbers are summed over the total orbital angular momentum of the atom, so the decomposition into final L' values is ignored, the phase shift is taken to be zero and $C_{\ell\ell'} = \ell_{>}/(2\ell + 1)$ where $\ell_{>}$ is the greater of ℓ and ℓ' . Electrons with orbital angular momentum $\ell' \geq 2$ in the final state have small phase shifts at low energies, so again the present calculation assumes the phase shift to vanish.

For photoionization of an outer electron to a final s or p state the zero energy phase shift is obtained by Eq. (5.12), extrapolating linearly from the physical bound

states with high principal quantum numbers. However, in the photoionization of an inner electron in the presence of an outer excited electron a difficulty occurs similar to that encountered for such states in the normalization procedure. Again, the physical states required are doubly-excited states and are unknown, so the extrapolation of the quantum defect is impossible. The present calculation sets the phase shift to zero for such states. Generally, the most significant low-energy phase shift is for final s-states, thus the $2p \rightarrow \epsilon s$ photoionization cross section in the presence of an outer excited electron is in question. However, the $2p \rightarrow \epsilon d$ transition, with small d-state phase shift, usually dominates the $2p \rightarrow \epsilon s$, so this uncertainty is probably not too great. A more serious difficulty is the neglect of the p-state phase shift in the $2s \rightarrow \epsilon p$ transition in the presence of the excited outer electron. The uncertainty due to this approximation can probably only be resolved by detailed electron scattering calculations or Hartree-Fock calculations of the continuum state.

A low-energy expansion of the Burgess-Seaton cross section, Eq. (5.6), for integer ν and to first order in ϵ agrees with a corresponding expansion of the exact hydrogenic results. Thus the Burgess-Seaton theory is to be considered a valid approximation when the electron kinetic energy is much less than Z^2 rydbergs. Furthermore, when sufficient information regarding the physical bound states is available, the result of Burgess and Seaton is probably more reliable than continuum Hartree-Fock calculations (Refs. 99 and 100) as some effects due to exchange and polarization of the core are reflected in the physical energies of the states with large principal quantum number used in the extrapolation for the phase shift.

Thus we conclude that the Burgess-Seaton approximation is a reasonably valid and useful approximation near the photoionization threshold, with the exception of the aforementioned inner-shell transitions in the presence of an excited outer electron. The simplicity of the resulting expression for the photoionization cross section renders it particularly suitable for evaluation of the large number of initial states present in this calculation.

THE HIGH-ENERGY THEORY

For energies of the final-state free electron much greater than zero the Burgess-Seaton approximation is inapplicable. An approximation of frequent utility in high-energy scattering calculations is the Born approximation. A straightforward application of the Born approximation to calculation of the photoionization cross section, however, leads to an incorrect result, as shown by Bethe and Salpeter (Ref. 91) in an hydrogenic calculation. Similar behavior has been noted by Kabir and Salpeter (Ref. 101) and by Dalgarno and Stewart (Ref. 102), who show that a Born approximation to the acceleration form of the photoionization matrix element yields a result asymptotically correct at high electron energies.

The basic expression for a radiative transition – in the electric-dipole approximation – between atomic states $|i\rangle$ and $|f\rangle$ is

$$\sigma_{fi} = \frac{4\pi^2 e^2 \omega}{c} |\langle f | \vec{r} | i \rangle|^2 \quad (5.13)$$

from which Eq. (5.3) is obtained upon performing the angular integrations and the average over the polarization directions of the incident radiation. As shown by Bethe and Salpeter (Ref. 91), forms equivalent to Eq. (5.13) are

$$\sigma_{fi} = \frac{4\pi^2 e^2}{m^2 c \omega} |\langle f | \vec{p} | i \rangle|^2 = \frac{4\pi^2 \bar{Z}^2 e^6}{m^2 c \omega^3} \left| \langle f | \frac{\vec{r}}{r^3} | i \rangle \right|^2 \quad (5.14)$$

the dipole-velocity and dipole-acceleration forms, respectively; \bar{Z} is the nuclear charge, m the electron mass. It can be shown (Ref. 103) that a use of the acceleration form of the matrix element in a high-energy Born approximation gains one iterate of the Born series over the use of the dipole-velocity form. The second Born approximation to the velocity matrix element contains a term with the same high-energy

behavior as the first-Born approximation – thus guaranteeing an incorrect high-energy result when using the first Born approximation alone – whereas the first Born approximation to the acceleration matrix element gives the correct high-energy behavior. Accordingly, the present calculation evaluates the photoionization cross section for high electron energy by the dipole-acceleration Born approximation.

When the angular integrations and polarization averages are performed in Eq. (5. 14), a result analogous to Eq. (5. 3) is obtained

$$\sigma_{ij}(\epsilon) = \frac{16\pi^3 Z^2 e^6}{3m^2 \omega^3 c} F_p \left[\left(\frac{l}{2l+1} \right) (R_{nl}^{\epsilon, l-1})^2 + \left(\frac{l+1}{2l+1} \right) (R_{nl}^{\epsilon, l+1})^2 \right] \quad (5. 15)$$

with

$$R_{nl}^{\epsilon l} = \int_0^{\infty} R_{\epsilon l}(r) \frac{1}{r^2} R_{nl}(r) r^2 dr \quad (5. 16)$$

In the first Born approximation the properly normalized free-electron wave function is the plane wave $-(k/2\pi^2)^{1/2} \exp(i\vec{k} \cdot \vec{r})$ – so

$$R_{nl}^{\epsilon l} = \sqrt{\frac{k}{2\pi^2}} \int_0^{\infty} j_l(kr) R_{nl}(r) dr \quad (5. 17)$$

in terms of the spherical Bessel functions $j_l(kr)$, where k^2 = electron kinetic energy in rydbergs.

Through use of a generalization of the HFS code of Hermann and Skillman (Ref. 104), wave functions have been generated for the many bound atomic states present in the gas. The resulting numerical wave functions have been fitted by analytic functions of the form

$$R_{nl}(r) = \sum_{n=1}^N C_n r^{\beta_n} e^{-\alpha_n r} \quad (5. 18)$$

with integer values of β_n . From comparison of the numerical results, the following conventions were adopted in order to reduce the number of orbitals required while still retaining accuracy suitable to the present application:

- (a) For ground-state cores - $2s^{n_s} 2p^{n_p} n\ell$, the orbital (n, ℓ) was calculated for $3 \leq n \leq 8$ and $\ell = 0, 1, 2, 3$ only. For all values of (n, ℓ) the core orbitals are approximated by those calculated with $(n = 3, \ell)$ unless $\ell = 3$, when the core orbitals used are those calculated with $(n = 4, \ell = 3)$.
- (b) For excited cores with one or more 2s-electrons excited to a 2p-orbit, the orbital (n, ℓ) is calculated for $n = 3, 4, 5$ and $\ell = 0, 1, 3$ and for $n = 3, 4$ for $\ell = 2$. For larger n the (n, ℓ) orbital is approximated by those calculated in the presence of the ground state core. The core orbitals are subject to the same conventions as in Case (a).

In terms of the bound orbitals, Eq. (5.18), Eq. (5.15) for the cross section becomes

$$\sigma_{nl}^{el'} = (1.712 \times 10^{-18}) \frac{\bar{Z}^2}{\omega^3 k} F_p C_{ll'} \left[\sum_{n=1}^N C_n \left(\frac{1}{k} \right)^n I_{l'} \left(\frac{\alpha_n}{k}, \beta_n \right) \right]^2 \text{ cm}^2 \quad (5.19)$$

where

$$C_{ll'} = (l'/2l + 1)$$

and

$$I_l(\alpha, \beta) = \int_0^\infty e^{-\alpha z} z^\beta j_l(z) dz$$

$$= \frac{\Gamma(\frac{1}{2})\Gamma(l + \beta + 1)}{2^{l+1}\Gamma(l + \frac{3}{2})} \frac{F\left(\frac{l + \beta + 1}{2}; \frac{l - \beta + 1}{2} \mid l + \frac{3}{2} \right)}{\left(1 + \alpha^2\right)^{1/2(l+\beta+1)}} \quad (5.20)$$

These are most easily evaluated using the recursion relations

$$\left. \begin{aligned}
 I_l(\alpha, \beta) &= \delta_{\beta 0} \delta_{l1} - \alpha I_{l-1}(\alpha, \beta) + (\beta + l - 1) I_{l-1}(\alpha, \beta - 1) \\
 I_0(\alpha, \beta) &= \Gamma(\beta) (1 + \alpha^2)^{-\beta/2} \sin [\beta \tan^{-1}(1/\alpha)] \\
 I_l(\alpha, 0) &= \delta_{l1} - \alpha \left(\frac{2l-1}{l} \right) I_{l-1}(\alpha, 0) - \left(\frac{l-1}{l} \right) I_{l-2}(\alpha, 0) \\
 I_0(\alpha, 0) &= \tan^{-1}(1/\alpha)
 \end{aligned} \right\} \quad (5.21)$$

As discussed by Chandrasekhar (Ref. 105) the three expressions [Eqs. (5.13) and (5.14)] are equivalent for exact wave functions but for approximate wave functions the fact that they weight different regions of configuration space differently leads to different results. Thus the Burgess-Seaton approximation of wave functions correct for large r starts from Eq. (5.13) and conforms to the familiar uncertainty-principle arguments that low-energy scattering states preferentially sample the long-range parts of the bound state. Similarly the high-energy scattering state weights more heavily the short-range part (the high-momentum Fourier components) of the bound state, as does the acceleration form of the matrix element. Variationally determined wave functions are usually less reliable for small than for intermediate values of r , so the accuracy at short distances of the HFS wave functions represents a source of uncertainty in the present results.

THE APPROXIMATE PHOTOIONIZATION CROSS SECTION

The occurrence of the spherical Bessel function in Eq. (5.17) represents an approximation to the more correct positive-energy regular Coulomb function valid if $k \gg Z$ - a domain of validity opposite to that of the Burgess-Seaton approximation, as discussed at the end of the first subsection. For the present calculation an exponential interpolation formula is utilized,

$$\sigma(\epsilon) = \sigma_{\text{BS}}(\epsilon) e^{-\alpha r} + \sigma_{\text{HE}}(\epsilon) [1 - e^{-\alpha r}] \quad (5.22)$$

where σ_{BS} and σ_{HE} are the photoionization cross sections calculated according to the Burgess-Seaton and high-energy approximations, respectively. The parameter α was chosen to weight the two approximations equally at $\epsilon = Z^2$ rydbergs.

Comparisons of the photoionization cross section obtained from Eq. (5.22) with Hartree-Fock calculations obtained with the computer program of Dalgarno, Henry, and Stewart (Ref. 100) are presented in Figs. V-1 through V-4. Included in the figures are results obtained by an hydrogenic approximation with Gaunt factors from Karzas and Latter (Ref. 89) and with the unit Gaunt factors used by Stewart and Pyatt (Ref. 8). It is seen that the hydrogenic approximation consistently underestimates the Hartree-Fock results and agreement improves for states of higher degree of ionization. Thus the hydrogenic approximation is most suitable at high temperatures and low densities. Comparing continuum Planck means obtained by Stewart and Pyatt with those of the present calculation - Sec. VI, Table VI-2 - bears out this observation.

The fact that the hydrogenic approximation to the photoionization cross section generally lies below that of Burgess and Seaton is consistent with the observation that the hydrogenic approximation assumes that the final-state free electron moves in a Coulomb field with the same effective charge as does the initial bound-state electron, whereas in the Burgess-Seaton approximation the free electron sees primarily the charge of the residual ion. The effective charge of the bound state is generally greater than the residual ionic charge, and this greater charge leads to a shorter-wavelength free-electron wave function and the resulting greater cancellation in the transition matrix element. Thus the replacement of the bound charge by the residual charge (the replacement of the hydrogenic by the Burgess-Seaton approximations) should decrease the cancellation and increase the magnitude of the cross section.

To account for bound-bound transitions with upper level above the merging limit, the photoionization cross section is extrapolated linearly to a value (Z^2/n_m^2) rydbergs below the vacuum edge, where n_m is defined in the discussion following Eq. (4.13) in Sec. IV.

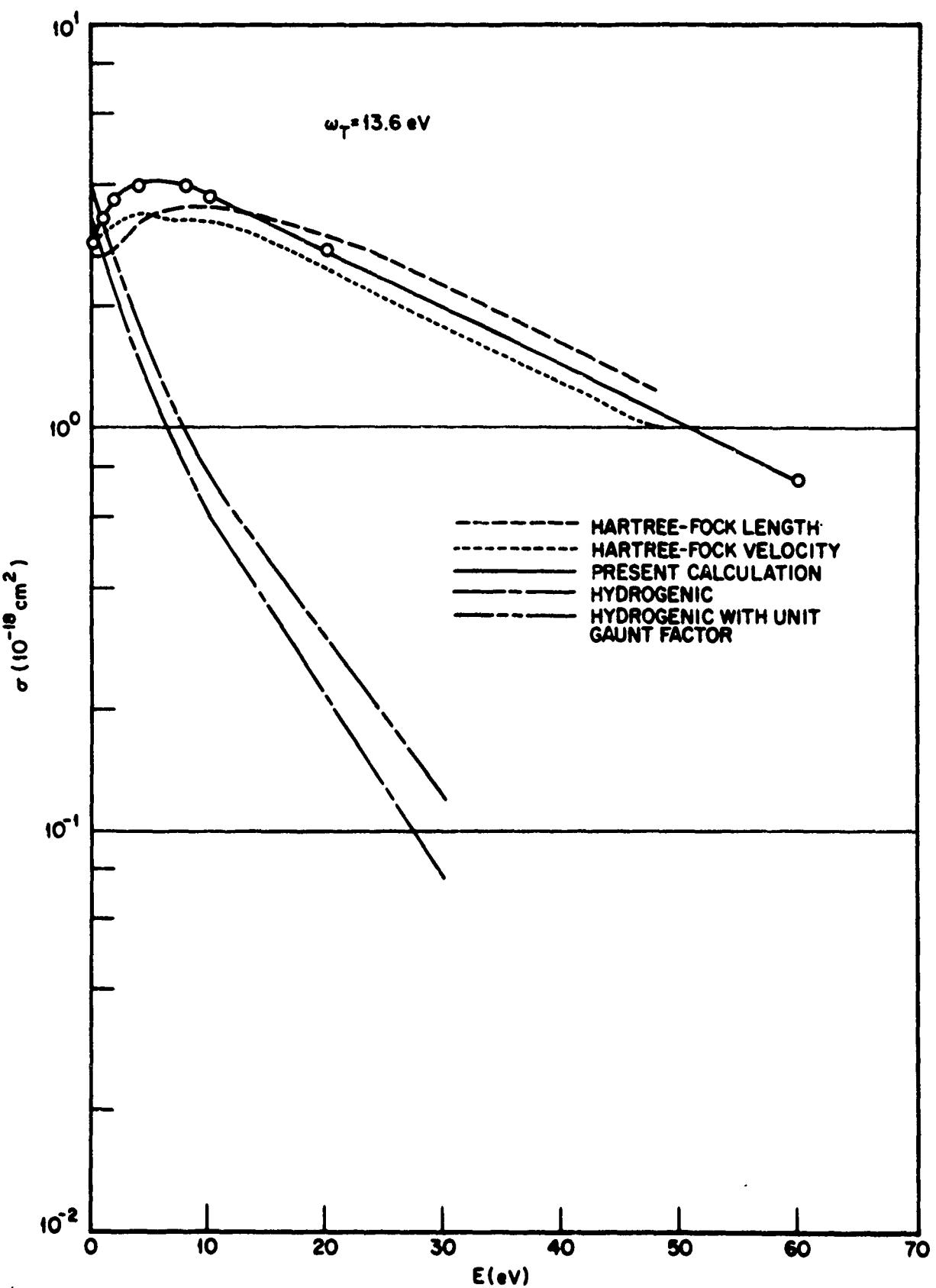


Fig. V-1 Comparison of photoionization cross section obtained with Hartree-Fock calculations of Ref. 100 and those obtained with Eq. (5.22) –
 OI: $2s^2 2p^4 (3P) \rightarrow 2s^2 2p^3 (4S) \epsilon$

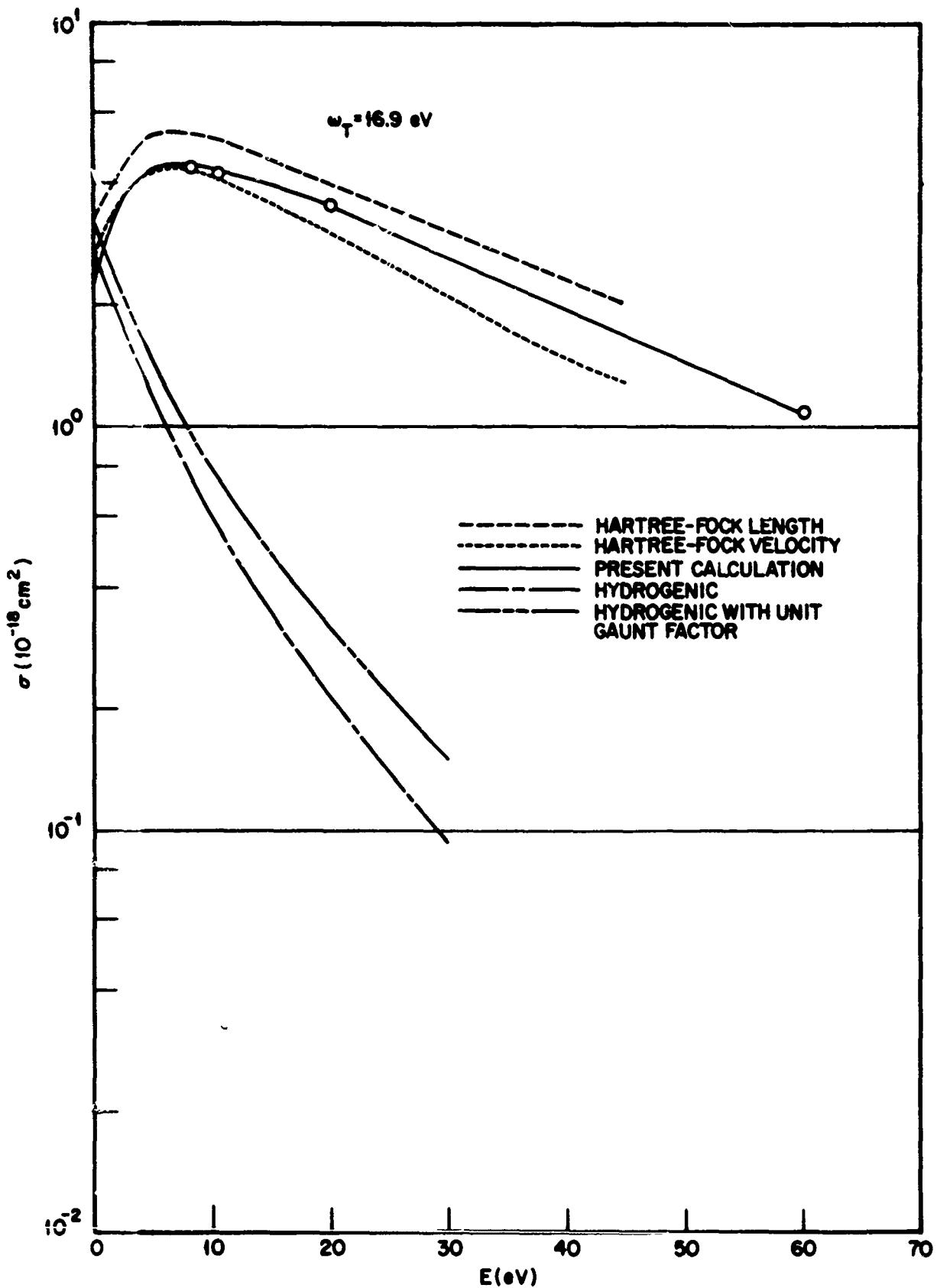


Fig. V-2 Comparison of photoionization cross section obtained with Hartree-Fock calculations of Ref. 100 and those obtained with Eq. (5.22) –
 $\text{OI: } 2s^2 2p^4 ({}^3P) \rightarrow 2s^2 2p^3 ({}^2D) e^-$

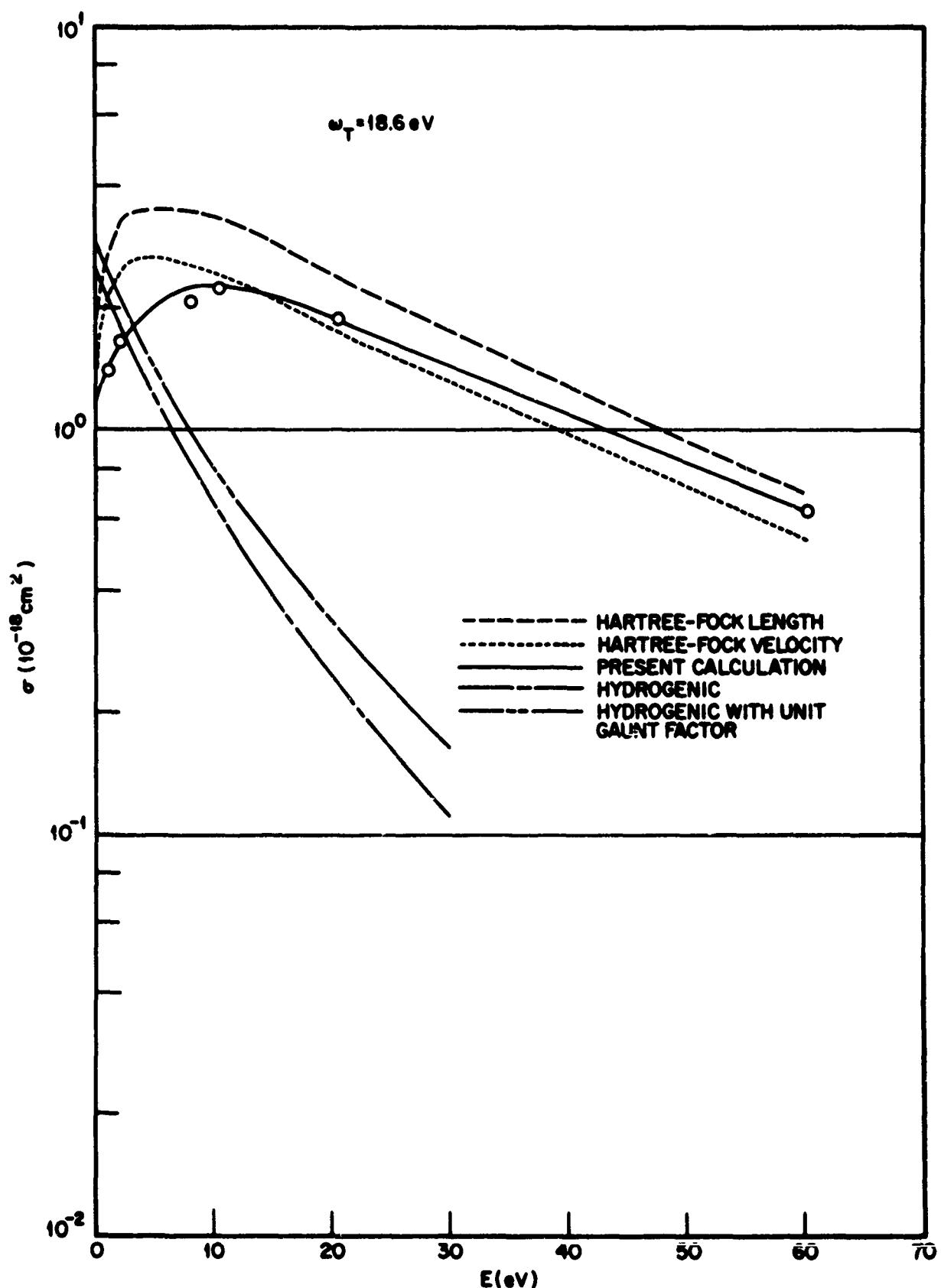


Fig. V-3 Comparison of photoionization cross section obtained with Hartree-Fock calculations of Ref. 100 and those obtained with Eq. (5.22) –
OI: $2s^2 2p^4 (3P) \rightarrow 2s^2 2p^3 (2P)$

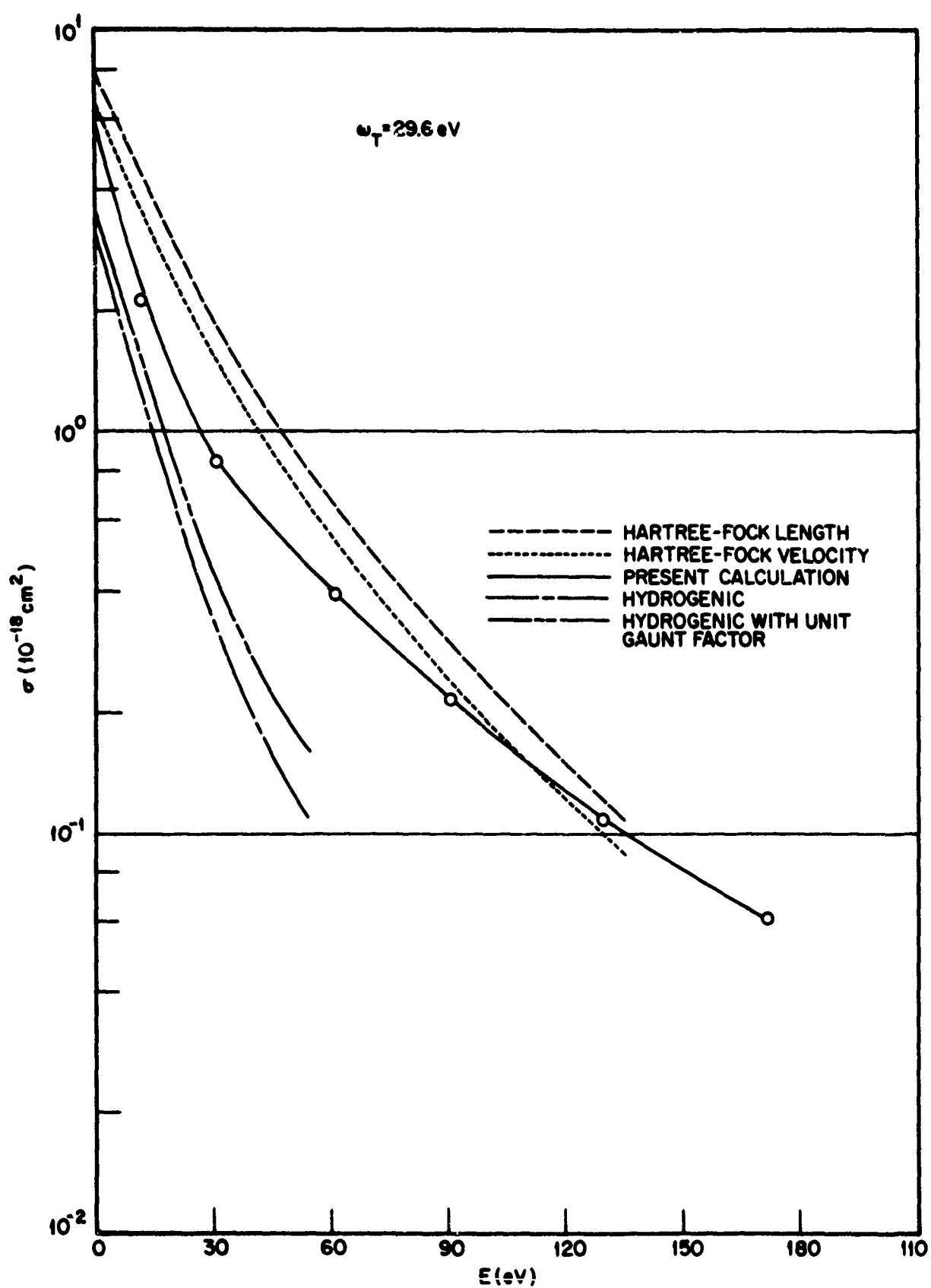


Fig. V-4 Comparison of photoionization cross section obtained with Hartree-Fock calculations of Ref. 100 and those obtained with Eq. (5.22) –
 NII: $2s^2 2p^2 (^3P) \rightarrow 2s^2 2p (^2P)\epsilon$

THE COMPUTER CODE PIC

A computer program PIC has been devised to compute the approximate photoionization cross section for each of the large number of atomic states present in the gas. The program is coded in the FORTRAN II (Version III) language and has been operated on an IBM-7094 computing system.

The initial data upon which the code operates are identical to those used by the program MULTIPLET, described in Sec. IV. For each atomic state one of whose occupation numbers is greater than an arbitrary cutoff α_0 — set equal to 10^{-5} for oxygen and for nitrogen — all possible photoionization transitions are computed by the approximations described in the preceding sections. For each transition the photoionization cross section is evaluated at a predetermined set of electron energies and the results are written onto a tape — generating an atlas of photoionization transitions.

The final phase of PIC is concerned with generating from the data in the photoionization atlas a frequency-dependent absorption coefficient $\mu(\epsilon)$, Eq. (5.1), over an arbitrary set of energies ϵ_N . For each desired set of equally-spaced energies the program is provided with a data card containing $(N_\omega, \omega_0, \Delta\omega)$, where $N_\omega (\leq 2000)$ is the number of energies at which the absorption coefficient is to be tabulated and $\epsilon_N = \omega_0 + (N - 1)\Delta\omega$, $(N = 1, N_\omega)$ specifies the energy set. For each transition in the photoionization atlas the cross section is evaluated at the energies ϵ_N and the continuous absorption coefficient [Eq. (5.1)] is accumulated.

A complete FORTRAN listing of PIC is included in Appendix C.

Section VI OPACITY RESULTS

CALCULATIONS

For purposes of radiation-transport calculations certain frequency averages of the radiation-absorption coefficient are of frequent utility. Two such mean opacities are considered here. The hydrogenic free-free absorption coefficients tabulated in Ref. 5 have been included in our results.

In emissivity studies the Planck mean opacity is a convenient result:

$$\bar{\mu}_P = \frac{15}{\pi^4 T^4} \int_0^{\infty} \epsilon^3 e^{-\epsilon/T} \mu(\epsilon) d\epsilon . \quad (6.1)$$

Results obtained for Planck mean opacities in the present calculation are presented in Table VI-1 for the temperatures and densities considered. The line contributions alone are in substantial agreement with the results of the preliminary calculation of Armstrong and Aroeste using the same f-numbers as used here (Ref. 106). As discussed in Ref. 106, the major discrepancy with the line Planck mean results of Stewart and Pyatt (Ref. 8) appears to be due to our inclusion of same-shell transitions. At the highest temperatures, however, where the Planck weighting function lessens the importance of these same-shell transitions it is found that our line Planck means fall consistently below those of Stewart and Pyatt. Part of this discrepancy is probably due to the effect noted in Sec. V that, in the non-hydrogenic approximations made here, part of the oscillator strength is squeezed out of the lines and into the continuum - relative to a hydrogenic approximation. However, the major source of the discrepancy is most likely due to our neglect of line transitions into doubly excited final states.

Table VI-1
PLANCK MEAN OPACITIES FOR NITROGEN AND OXYGEN

Temperature (eV)	J	Nitrogen Ion Density (nuclei cm ⁻³)	Mean Opacity (cm ⁻¹)			Oxygen Ion Density (nuclei cm ⁻³)	Mean Opacity (cm ⁻¹)		
			Lines	Continuum	Total		Lines	Continuum	Total
1	1	5.25 ¹⁸	1.70	3.48 ⁻²	1.74	5.38 ¹⁸	5.20 ⁻¹	2.04 ⁻²	5.40 ⁻¹
	2	5.36 ¹⁷	1.68 ⁻¹	3.40 ⁻³	1.71 ⁻¹	5.39 ¹⁷	4.67 ⁻²	1.82 ⁻³	4.85 ⁻²
	3	5.37 ¹⁶	1.51 ⁻²	2.84 ⁻⁴	1.54 ⁻²	5.37 ¹⁶	4.22 ⁻³	1.60 ⁻⁴	4.38 ⁻³
	4	5.38 ¹⁵	1.10 ⁻³	1.71 ⁻⁵	1.12 ⁻³	5.38 ¹⁵	3.09 ⁻⁴	1.13 ⁻⁵	3.20 ⁻⁴
	5	5.38 ¹⁴	5.89 ⁻⁵	5.27 ⁻⁷	5.94 ⁻⁵	5.38 ¹⁴	1.37 ⁻⁵	3.53 ⁻⁷	1.41 ⁻⁵
	6	5.38 ¹³	3.90 ⁻⁶	6.61 ⁻⁹	3.91 ⁻⁶	5.38 ¹³	5.41 ⁻⁷	5.51 ⁻⁹	5.47 ⁻⁷
2	1	2.34 ²⁰	8.04 ²	1.61 ²	9.65 ²	3.32 ²⁰	5.16 ²	1.61 ²	6.77 ²
	2	3.16 ¹⁸	6.61	4.01 ⁻¹	7.01	3.77 ¹⁸	3.21	4.19 ⁻¹	3.63
	3	3.32 ¹⁷	6.06 ⁻¹	7.20 ⁻³	6.13 ⁻¹	3.85 ¹⁷	2.67 ⁻¹	6.97 ⁻³	2.74 ⁻¹
	4	3.86 ¹⁶	6.75 ⁻²	1.92 ⁻⁴	6.77 ⁻²	4.68 ¹⁶	3.09 ⁻²	1.31 ⁻⁴	3.10 ⁻²
	5	3.90 ¹⁵	6.18 ⁻³	6.21 ⁻⁶	6.19 ⁻³	5.59 ¹⁵	3.57 ⁻³	3.23 ⁻⁶	3.57 ⁻³
	6	3.97 ¹⁴	5.41 ⁻⁴	1.43 ⁻⁷	5.41 ⁻⁴	5.59 ¹⁴	3.20 ⁻⁴	9.71 ⁻⁸	3.20 ⁻⁴
5	1	2.56 ²⁰	1.20 ³	2.32 ²	1.43 ³	3.02 ²⁰	1.05 ³	2.01 ²	1.25 ³
	2	5.50 ¹⁸	1.99 ¹	7.97 ⁻¹	2.07 ¹	6.57 ¹⁸	1.83 ¹	6.73 ⁻¹	1.90 ¹
	3	5.24 ¹⁷	1.50	2.11 ⁻²	1.52	6.45 ¹⁷	1.61	1.96 ⁻²	1.63
	4	5.65 ¹⁶	1.28 ⁻¹	4.75 ⁻⁴	1.29 ⁻¹	6.76 ¹⁶	1.50 ⁻¹	5.16 ⁻⁴	1.51 ⁻¹
	5	6.49 ¹⁵	1.09 ⁻²	8.99 ⁻⁶	1.09 ⁻²	7.97 ¹⁵	1.67 ⁻²	9.64 ⁻⁶	1.67 ⁻²
	6	7.50 ¹⁴	7.02 ⁻⁴	1.64 ⁻⁷	7.02 ⁻⁴	9.25 ¹⁴	1.80 ⁻³	1.96 ⁻⁷	1.80 ⁻³
10	1	4.11 ²⁰	9.14 ²	2.87 ²	12.01 ²	4.76 ²⁰	1.16 ³	3.11 ²	1.47 ³
	2	8.81 ¹⁸	0.99 ¹	8.15 ⁻¹	1.07	1.04 ¹⁹	1.63 ¹	1.07	1.74 ¹
	3	8.71 ¹⁷	4.31 ⁻¹	1.72 ⁻²	4.48 ⁻¹	1.03 ¹⁸	9.78 ⁻¹	2.50 ⁻³	1.00
	4	9.79 ¹⁶	1.16 ⁻²	3.40 ⁻⁴	1.19 ⁻²	1.11 ¹⁷	5.08 ⁻²	5.81 ⁻⁴	5.14 ⁻²
	5	1.23 ¹⁶	2.25 ⁻⁴	5.36 ⁻⁶	2.30 ⁻⁴	1.29 ¹⁶	2.98 ⁻³	1.08 ⁻⁵	2.37 ⁻³
	6	1.62 ¹⁵	4.09 ⁻⁶	8.02 ⁻⁸	4.17 ⁻⁶	1.58 ¹⁵	6.63 ⁻⁵	1.65 ⁻⁷	6.65 ⁻⁵
15	1	5.53 ²⁰	6.05 ²	2.42 ²	8.47 ²	6.40 ²⁰	9.62 ²	3.33 ²	1.30 ³
	2	1.27 ¹⁹	3.72	5.54 ⁻¹	4.27	1.42 ¹⁹	1.07 ¹	9.61 ⁻¹	1.17 ¹
	3	1.39 ¹⁸	7.51 ⁻²	9.38 ⁻³	8.45 ⁻²	1.44 ¹⁸	4.20 ⁻¹	1.96 ⁻²	4.40 ⁻¹
	4	1.72 ¹⁷	1.34 ⁻³	1.60 ⁻⁴	1.50 ⁻³	1.68 ¹⁷	9.98 ⁻³	3.65 ⁻⁴	1.03 ⁻²
	5	2.23 ¹⁶	2.42 ⁻⁵	2.68 ⁻⁶	2.69 ⁻⁵	2.14 ¹⁶	1.87 ⁻⁴	5.98 ⁻⁶	1.93 ⁻⁴
	6	2.96 ¹⁵	4.39 ⁻⁷	4.32 ⁻⁸	4.82 ⁻⁷	2.83 ¹⁵	3.41 ⁻⁶	8.00 ⁻⁸	3.50 ⁻⁶
20	1	7.07 ²⁰	3.42 ²	1.87 ²	5.29 ²	8.01 ²⁰	7.02 ²	3.04 ²	1.01 ³
	2	1.90 ¹⁹	1.21	3.58 ⁻¹	1.57	1.88 ¹⁹	5.45	7.10 ⁻¹	6.16
	3	2.08 ¹⁸	2.12 ⁻²	5.72 ⁻³	2.69 ⁻²	2.04 ¹⁸	1.21 ⁻¹	1.23 ⁻²	1.33 ⁻¹
	4	2.62 ¹⁷	3.71 ⁻⁴	9.78 ⁻⁵	4.69 ⁻⁴	2.52 ¹⁷	2.16 ⁻³	2.11 ⁻⁴	2.37 ⁻³
	5	3.42 ¹⁶	6.52 ⁻⁶	1.70 ⁻⁶	5.32 ⁻⁶	3.27 ¹⁶	3.38 ⁻⁵	3.62 ⁻⁶	4.22 ⁻⁵
	6	4.55 ¹⁵	1.23 ⁻⁷	2.82 ⁻⁸	1.51 ⁻⁷	4.34 ¹⁵	6.96 ⁻⁷	5.64 ⁻⁸	7.52 ⁻⁷

In Table VI-2 are comparisons of our results for continuum Planck mean opacities – photoelectric plus hydrogenic free-free – with the earlier hydrogenic results of Armstrong (Ref. 5) which used the same initial atomic states and occupations thereof as used here. Thus the present calculation differs from that of Armstrong primarily in the use of nonhydrogenic matrix elements. It is seen that the present results lie consistently above the earlier hydrogenic values. Included in Table VI-2 are the nitrogen continuum Planck means of Stewart and Pyatt (Ref. 8) interpolated to our densities. (The 20-eV Stewart-Pyatt data are the result of a double interpolation in both density and temperature and are thus somewhat less reliable.) The Stewart and Pyatt calculation is also an hydrogenic approximation with unit Gaunt factors. The occupation numbers were obtained by a theoretical approximation different from ours.

The present calculation of the line Planck mean opacity numerically integrates the accumulated line absorption coefficient due to broad lines and, for each narrow line, accumulates the Planck integrand [Eq. (6.1)] at the position of each narrow line. The distinction between broad and narrow lines is discussed at the conclusion of Sec. IV.

A frequency-averaged absorption coefficient useful in radiation diffusion calculations is the Rosseland mean free path

$$\lambda_R \equiv \bar{\mu}_R \equiv \frac{1}{4\pi T^5} \int_0^\infty \frac{\epsilon^4 \exp(2\epsilon/T) d\epsilon}{\mu(\epsilon) [\exp(\epsilon/T) - 1]^3} \quad (6.2)$$

where $\bar{\mu}_R$ is the Rosseland mean opacity. Our results for the Rosseland mean opacities are presented in Table VI-3, which includes for comparison the nitrogen results of Stewart and Pyatt (Ref. 8). Compton scattering has been included in our results (for the Rosseland, not the Planck mean) and K-shell effects are neglected.

The Rosseland mean opacity [Eq. (6.2)] – being an inverse mean of the absorption coefficient $\mu(E)$ – is a non-additive function of the line, photoionization, free-free, and scattering contributions to the absorption coefficient. Therefore, a modified version of the final phase of MULTIPLET has been devised – the code RABS, a complete FORTRAN listing of which is included in Appendix D.

Table VI-2
CONTINUUM PLANCK MEAN OPACITIES FOR NITROGEN AND OXYGEN
COMPARISON WITH PREVIOUS RESULTS

Temperature (eV)	J	Nitrogen Mean Opacity (cm ⁻¹)			Oxygen Mean Opacity (cm ⁻¹)	
		Present Calculation	Ref. 5	Ref. 8	Present Calculation	Ref. 5
2	1	1.61 ²	1.28 ²		1.61 ²	1.08 ²
	2	4.01 ⁻¹	3.00 ⁻¹		4.19 ⁻¹	2.81 ⁻¹
	3	7.20 ⁻³	4.99 ⁻³		6.97 ⁻³	4.60 ⁻³
	4	1.92 ⁻⁴	1.05 ⁻⁴		1.31 ⁻⁴	8.11 ⁻⁵
	5	6.21 ⁻⁶	2.98 ⁻⁶		3.23 ⁻⁶	1.82 ⁻⁶
	6	1.43 ⁻⁷	7.08 ⁻⁸		9.71 ⁻⁸	5.82 ⁻⁸
5	1	2.32 ²	1.70 ²	1.1 ²	2.01 ²	1.52 ²
	2	7.97 ⁻¹	3.87 ⁻¹	3.5 ⁻¹	6.73 ⁻¹	5.03 ⁻¹
	3	2.11 ⁻²	8.58 ⁻³	8.4 ⁻³	1.98 ⁻²	7.61 ⁻³
	4	4.75 ⁻⁴	1.69 ⁻⁴	1.9 ⁻⁴	5.16 ⁻⁴	1.68 ⁻⁴
	5	8.99 ⁻⁶	3.85 ⁻⁶	4.1 ⁻⁶	9.64 ⁻⁶	3.50 ⁻⁶
	6	1.64 ⁻⁷	8.99 ⁻⁸	9.1 ⁻⁸	1.96 ⁻⁷	8.42 ⁻⁸
10	1	2.87 ²	2.12 ²	1.3 ²	3.11 ²	2.14 ²
	2	8.15 ⁻¹	4.63 ⁻¹	3.8 ⁻¹	1.07	4.66 ⁻¹
	3	1.72 ⁻²	9.13 ⁻³	9.0 ⁻³	2.50 ⁻²	9.77 ⁻³
	4	3.40 ⁻⁴	1.79 ⁻⁴	1.9 ⁻⁴	5.81 ⁻⁴	2.02 ⁻⁴
	5	5.36 ⁻⁶	3.25 ⁻⁶	3.4 ⁻⁶	1.08 ⁻⁵	3.78 ⁻⁶
	6	8.02 ⁻⁸	5.81 ⁻⁸	6.0 ⁻⁸	1.65 ⁻⁷	7.11 ⁻⁸
15	1	2.42 ²	2.11 ²	1.2 ²	3.33 ²	2.28 ²
	2	5.54 ⁻¹	3.84 ⁻¹	3.2 ⁻¹	9.61 ⁻¹	4.68 ⁻¹
	3	9.38 ⁻³	6.50 ⁻³	6.2 ⁻³	1.95 ⁻²	8.59 ⁻³
	4	1.60 ⁻⁴	1.03 ⁻⁴	1.1 ⁻⁴	3.65 ⁻⁴	1.35 ⁻⁴
	5	2.68 ⁻⁶	1.79 ⁻⁶	1.9 ⁻⁶	5.98 ⁻⁶	2.34 ⁻⁶
	6	4.32 ⁻⁸	3.16 ⁻⁸	3.4 ⁻⁸	8.89 ⁻⁸	4.19 ⁻⁸
20	1	1.87 ²	1.61 ²	1.2 ²	3.04 ²	2.15 ²
	2	3.58 ⁻¹	2.30 ⁻¹	3.0 ⁻¹	7.10 ⁻¹	3.66 ⁻¹
	3	5.72 ⁻³	3.48 ⁻³	5.9 ⁻³	1.23 ⁻²	5.96 ⁻³
	4	9.78 ⁻⁵	5.66 ⁻⁵	1.1 ⁻⁴	2.11 ⁻⁴	9.26 ⁻⁵
	5	1.70 ⁻⁶	9.90 ⁻⁷	2.0 ⁻⁶	3.62 ⁻⁶	1.60 ⁻⁶
	6	2.82 ⁻⁸	1.75 ⁻⁸	3.6 ⁻⁸	5.64 ⁻⁸	2.81 ⁻⁸

Table VI-3

ROSSELAND MEAN OPACITIES FOR NITROGEN, OXYGEN, AND AIR

Temperature (eV)	Nitrogen Ion Density (nuclei cm ⁻³)	Mean Opacity (cm ⁻¹)		Oxygen Ion Density (nuclei cm ⁻³)	LMSC Mean Opacity (cm ⁻¹)	Air Ion Density (nuclei cm ⁻³)	LMSC Mean Opacity (cm ⁻¹)
		LMSC	Ref. 8				
1	5.25 ¹⁸	1.22 ⁻³		5.38 ¹⁸	2.48 ⁻³	5.28 ¹⁸	
	5.36 ¹⁷	1.10 ⁻⁴		5.39 ¹⁷	1.78 ⁻⁴	5.37 ¹⁷	
	5.37 ¹⁶	9.13 ⁻⁶		5.37 ¹⁶	1.47 ⁻⁵	5.37 ¹⁶	
	5.38 ¹⁵	5.40 ⁻⁷		5.38 ¹⁵	9.36 ⁻⁷	5.38 ¹⁵	
	5.38 ¹⁴	1.56 ⁻⁸		5.38 ¹⁴	2.93 ⁻⁸	5.38 ¹⁴	
	5.38 ¹³	2.06 ⁻¹⁰		5.38 ¹³	3.74 ⁻¹⁰	5.38 ¹³	
2	2.34 ²⁰	8.68 ¹		3.32 ²⁰	1.18 ²	2.55 ²⁰	9.78 ¹
	3.16 ¹⁸	1.16 ⁻¹		3.77 ¹⁸	2.27 ⁻¹	3.29 ¹⁸	1.52 ⁻¹
	3.32 ¹⁷	1.07 ⁻³		3.85 ¹⁷	1.47 ⁻³	3.43 ¹⁷	1.24 ⁻³
	3.86 ¹⁶	1.97 ⁻⁵		4.68 ¹⁶	2.35 ⁻⁵	4.03 ¹⁶	2.09 ⁻⁵
	3.90 ¹⁵	5.58 ⁻⁷		5.59 ¹⁵	3.26 ⁻⁷	4.26 ¹⁵	5.19 ⁻⁷
	3.97 ¹⁴	1.19 ⁻⁸		5.59 ¹⁴	4.10 ⁻⁹	4.31 ¹⁴	1.06 ⁻⁸
5	2.56 ²⁰	2.81 ²	1.5 ²	3.02 ²⁰	2.62 ²	2.66 ²⁰	3.35 ²
	5.50 ¹⁸	5.15 ⁻¹	3.2 ⁻¹	6.57 ¹⁸	4.10 ⁻¹	5.73 ¹⁸	6.05 ⁻¹
	5.24 ¹⁷	6.35 ⁻³	6.3 ⁻³	6.45 ¹⁷	5.96 ⁻³	5.50 ¹⁷	6.92 ⁻³
	5.65 ¹⁶	1.06 ⁻⁴	1.0 ⁻⁴	6.76 ¹⁶	9.61 ⁻⁵	5.88 ¹⁶	1.12 ⁻⁴
	6.49 ¹⁵	1.67 ⁻⁶	1.8 ⁻⁶	7.97 ¹⁵	1.45 ⁻⁶	6.80 ¹⁵	1.76 ⁻⁶
	7.50 ¹⁴	2.41 ⁻⁸	3.6 ⁻⁸	9.25 ¹⁴	1.99 ⁻⁸	7.87 ¹⁴	2.51 ⁻⁸
10	4.11 ²⁰	6.92 ²	3.4 ²	4.76 ²⁰	3.20 ²	4.25 ²⁰	7.78 ²
	8.81 ¹⁸	1.01	7.3 ⁻¹	1.04 ¹⁹	7.97 ⁻¹	9.14 ¹⁸	1.09
	8.71 ¹⁷	1.04 ⁻²	9.6 ⁻³	1.03 ¹⁸	1.02 ⁻²	9.04 ¹⁷	1.16 ⁻²
	9.79 ¹⁶	1.27 ⁻⁴	1.2 ⁻⁴	1.11 ¹⁷	1.69 ⁻⁴	1.01 ¹⁷	1.47 ⁻⁴
	1.23 ¹⁶	1.67 ⁻⁶	1.5 ⁻⁶	1.29 ¹⁶	2.96 ⁻⁶	1.25 ¹⁶	2.15 ⁻⁶
	1.62 ¹⁵	2.95 ⁻⁸	2.9 ⁻⁸	1.58 ¹⁵	4.36 ⁻⁸	1.61 ¹⁵	3.84 ⁻⁸
15	5.53 ²⁰	4.19 ²	2.5 ²	6.40 ²⁰	7.73 ²	5.72 ²⁰	5.50 ²
	1.27 ¹⁹	6.55 ⁻¹	6.3 ⁻¹	1.42 ¹⁹	1.08	1.30 ¹⁹	8.46 ⁻¹
	1.39 ¹⁸	5.48 ⁻³	5.8 ⁻³	1.44 ¹⁸	1.12 ⁻²	1.40 ¹⁸	8.01 ⁻³
	1.72 ¹⁷	7.01 ⁻⁵	5.9 ⁻⁵	1.68 ¹⁷	1.34 ⁻⁴	1.71 ¹⁷	1.04 ⁻⁴
	2.23 ¹⁶	1.16 ⁻⁶	9.8 ⁻⁷	2.14 ¹⁶	1.85 ⁻⁶	2.22 ¹⁶	1.66 ⁻⁶
	2.98 ¹⁵	3.17 ⁻⁸	3.2 ⁻⁸	2.83 ¹⁵	3.78 ⁻⁸	2.94 ¹⁵	3.88 ⁻⁸
20	7.07 ²⁰	1.87 ²	1.6 ²	8.01 ²⁰	5.42 ²	7.27 ²⁰	2.84 ²
	1.80 ¹⁹	3.15 ⁻¹	5.0 ⁻¹	1.86 ¹⁹	7.44 ⁻¹	1.81 ¹⁹	5.14 ⁻¹
	2.08 ¹⁸	3.67 ⁻³	6.1 ⁻³	2.04 ¹⁸	6.30 ⁻³	2.07 ¹⁸	5.80 ⁻³
	2.62 ¹⁷	5.74 ⁻⁵	6.9 ⁻⁵	2.52 ¹⁷	8.01 ⁻⁵	2.55 ¹⁷	6.31 ⁻⁵
	3.42 ¹⁶	1.11 ⁻⁶	1.2 ⁻⁶	3.27 ¹⁶	1.35 ⁻⁶	3.39 ¹⁶	1.59 ⁻⁶
	4.55 ¹⁵	3.58 ⁻⁸	4.2 ⁻⁸	4.34 ¹⁵	4.04 ⁻⁸	4.51 ¹⁵	4.35 ⁻⁸

The program RABS is identical to Phase 3 of MULTIPLET with the modification that prior to accumulating the broad-line contribution to the absorption coefficient the hydrogenic free-free absorption coefficient from Ref. 5 is read from cards, the tabulated photoionization coefficient from the code PIC (Sec. V) is read from tape, and the Compton scattering cross section is calculated. The broad-line absorption coefficient is then accumulated on top of these continuum contributions.

For the purposes of the Rosseland-mean calculation the narrow lines are divided into two classes - strong and weak. Strong lines are those whose strength at the line center is greater than the continuous absorption coefficient - evaluated at the line center; the remaining narrow lines are classified as weak. In RABS the line wings of the strong narrow lines are accumulated with the broad lines, so the final tape resulting from RABS contains the tabulated absorption coefficient due to all atomic contributions except the weak narrow lines and the line centers of the strong narrow lines.

To finally evaluate the Rosseland mean opacity, a computer program ROSS is utilized to read the tape provided by RABS and to properly accumulate the narrow-line contribution to the local mean free path - averaged over the small frequency interval $\Delta\omega$ (defined at the end of Sec. IV). The local mean free path is tabulated by the code as a function of energy and density; a numerical integration of Eq. (6.2) - with a variable upper limit - is carried out, and the code tabulates the resulting partial Rosseland means.

The mean free path frequency-averaged over the small interval $\Delta\omega$ is calculated by attributing a rectangular shape to the weak narrow lines and a Lorentz shape to the strong narrow lines. The frequency interval $\Delta\omega$ is then subdivided into generally unequal subintervals sufficient to adequately represent numerically the narrow lines in the interval. Over these refined subintervals the narrow lines are accumulated with the rest of the absorption coefficient and the local mean free path is obtained by numerical integration. A complete FORTRAN listing of ROSS is included in Appendix D.

COMPARISON WITH EXPERIMENT

An experimental observation of the emissivity of pure nitrogen at a temperature of 11,000°K and a density 1.16×10^{-2} normal has recently been carried out by Boldt (Ref. 107). The intensity measurements covered a wavelength interval of 4000 to 6000 Å, and the effects due to strong narrow lines were omitted. A comparison of the results of our calculation at Boldt's temperature and density with the experimental results is shown in Fig. VI-1. Included are our line emissivities, averaged over 200-Å intervals and not corrected for self-absorption. It is seen that most of the emissivity is due to photoionization transitions.

Allen* and associates at AVCO (Ref. 108) have recently measured the emissivity of an air sample at a temperature of 10,500°K and normal density over a wavelength interval 0.5 to 1.3 μ . (5000 to 13,000 Å.) The total emitted intensity is observed over 50-Å intervals from 0.5 to 0.6 μ and over 300-Å intervals from 0.8 to 1.3 μ . The experimental results and our theoretical approximations thereto are presented in Fig. VI-2.

Our nitrogen calculation was carried out in fair detail with an approximate correction for self-absorption of the strong narrow lines by limiting their intensity to the theoretical maximum, the Planck function. The oxygen calculation was quite crude in that multiplet splitting of the 3s and 3p states was ignored. Thus the 3s and 3p transitions which dominate the region 0.7 to 1 μ appeared at a single energy, whereas, in fact, they should be spread over an 1800-Å interval. In view of the crudeness of the oxygen treatment and our uncertainty in matching the experimental conditions, our results are in reasonable agreement with the experimental data.

CONCLUSIONS

As indicated in the introduction, the aim of the present study was to remove those hydrogenic approximations most seriously in question in previous calculations and to

*Private communication.

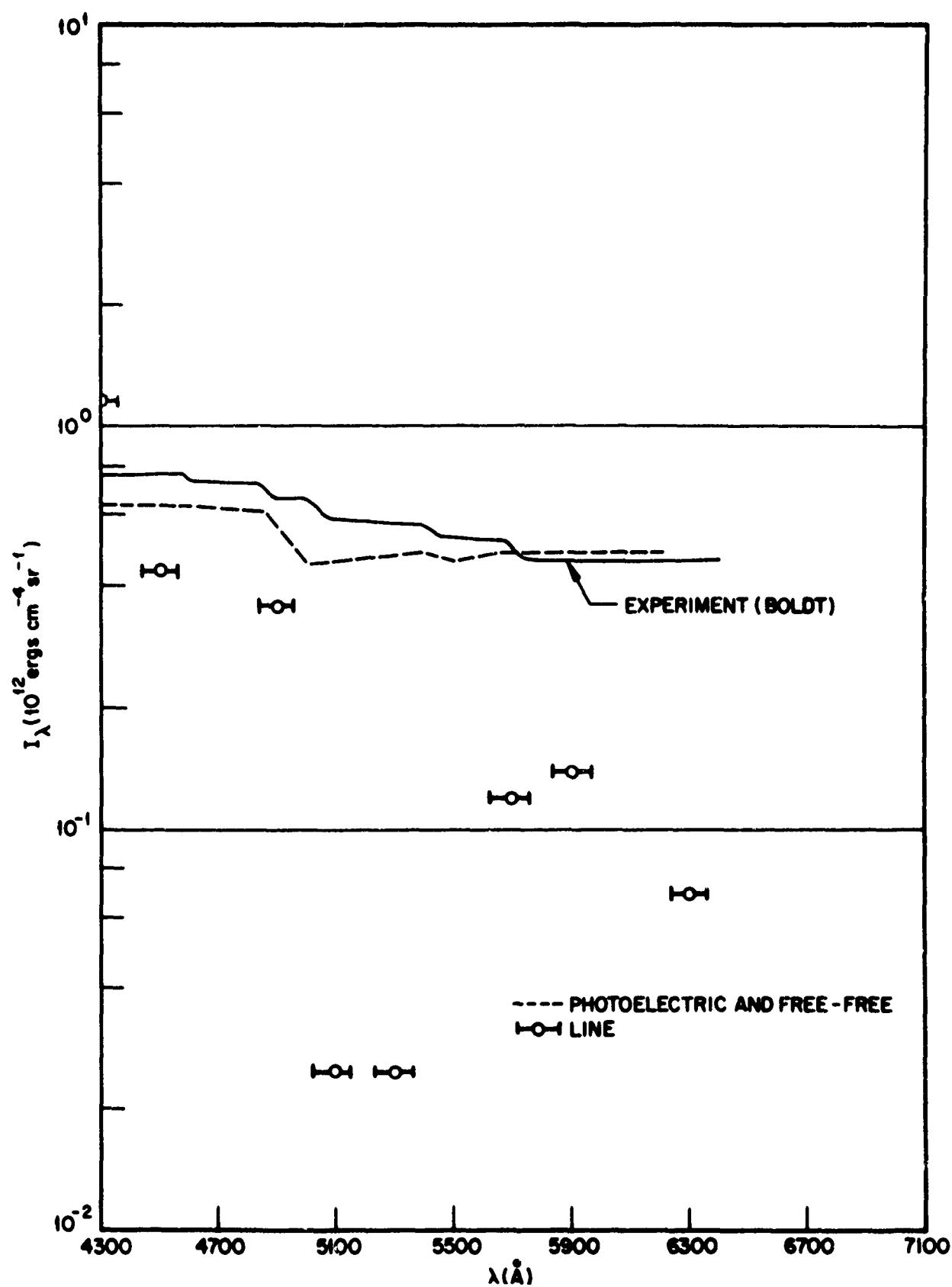


Fig. VI-1 Comparison of experimental data from Ref. 107 with the results of the present calculations.

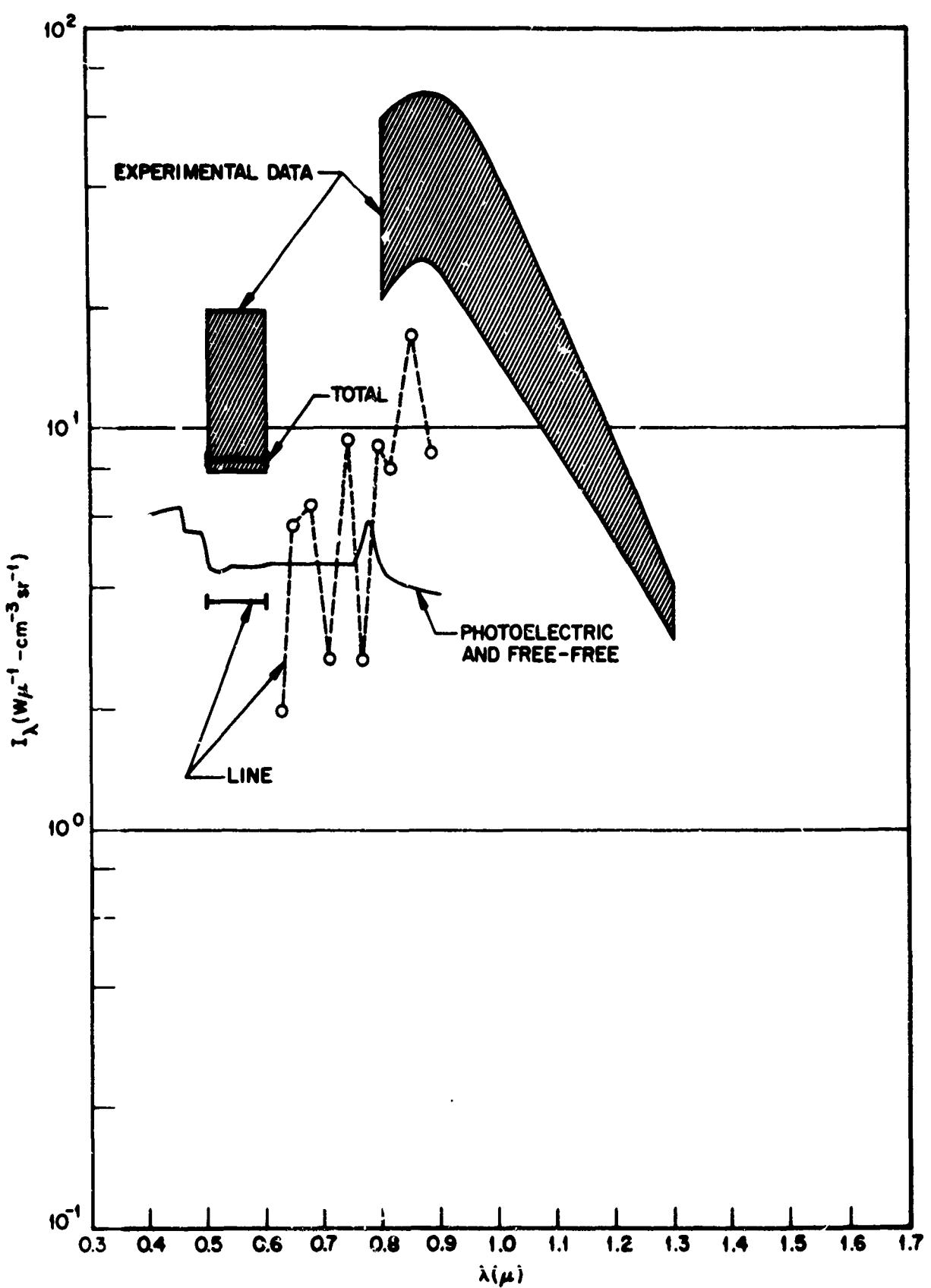


Fig. VI-2 Comparison of experimental data from Ref. 108 with the results of the present calculations.

study the effects thereof. To this end the bulk of the hydrogenic matrix elements have been replaced by physically more reasonable values, and computer programs have been developed to treat the relevant physical processes in as much detail as practicable, consistent with the uncertainties in the basic physical parameters. Some mean opacities useful in radiative transfer problems have been evaluated, and, by use of the computer programs, more detailed results are easily obtainable.

It is felt that the major source of uncertainty in our results is likely to be our neglect of line transitions to doubly-excited final atomic states. The effect of this neglect is undoubtedly showing up in our line Planck mean results. Due to the overlap of such final states with the continuum the states are subject to autoionization and thus should be quite broad – affecting the Rosseland mean opacities. An adequate treatment of such transitions would require a detailed theoretical study of the broadening problem.

The lack of experimental information regarding these same doubly-excited states forces some rather arbitrary approximations in the Burgess-Seaton calculation of the photoionization of inner electrons – as discussed in Sec. V. A noticeable improvement would probably require more detailed and time-consuming Hartree-Fock calculations similar to those of Dalgarno (Ref. 100).

At low photon energies and high temperatures the free-free absorption becomes a significant contribution to the opacity. The hydrogenic values used in this work are certainly subject to doubt and further studies of nonhydrogenic approximations are undoubtedly warranted for the free-free contribution.

In view of the accuracy of our input information and the amount of physical detail we have taken into account we feel that our results should be the most accurate air opacity results presented to date. However, we cannot place quantitative estimates on our accuracy, as this project has of necessity had to be terminated before the requisite analysis could be carried out. Detailed parameter studies and numerical estimates of neglected effects should be undertaken as well as further checking and testing of our results.

Appendix A STATISTICAL MECHANICS OF PLASMAS*

A. 1 GENERALIZATION OF SIEGERT'S DERIVATION OF THE OCCUPATION NUMBER FORMULA

It appears that the variational derivation given by Siegert of the formula for the occupation number, N_z^*, J_z , [Ref. 4, Eq. (20)], can be improved somewhat. Furthermore, it is worthwhile to consider the derivation of this and related formulas from a different approach, namely use of the grand canonical partition function. There are at least two reasons for looking at this alternative derivation. First in the framework of the grand partition function it is easy to include electron-degeneracy effects due to the operation of Fermi statistics. Secondly, results for the interaction free energy including quantum effects for a dense plasma are usually obtained using the grand partition function.

One-component Plasma Using the Grand Partition Function. To illustrate a few points that will come up in the treatment of an ionized gas, we first look at the electron gas in a smeared-out positive background. The grand partition function is

$$Z_G(\alpha, \beta) \equiv e^{\beta\Omega} = \text{Tr} \exp \left\{ \alpha N - \beta \left(H_0 + \frac{1}{2} \sum_{i \neq j}^N \frac{e^2}{r_{ij}} \right) \right\}.$$

Recall that the thermodynamic potential Ω is identical to the pressure $\Omega \equiv PV$, but as a function of α and β , not ρ and β . The two parameters, α = chemical

*This appendix was written by H. E. DeWitt.

potential and $\beta = 1/kT$, are normalized to the number of particles and the energy respectively, as obtained from

$$\bar{E} = -\frac{\partial(\beta\Omega)}{\partial\beta} = \frac{\text{Tr } H \exp(\alpha N - \beta H)}{\text{Tr } \exp(\alpha N - \beta H)}$$

$$\bar{N} = \frac{\partial(\beta\Omega)}{\partial\beta} = \frac{\text{Tr } N \exp(\alpha N - \beta H)}{\text{Tr } \exp(\alpha N - \beta H)}$$

$\beta\Omega_I$ is the interaction contribution to the grand potential. For the electron gas of any degree of degeneracy we have

$$\beta\Omega = \bar{N} \frac{\mathcal{J}_{3/2}(\alpha)}{\zeta} + \beta\Omega_I$$

where

$$\zeta = \frac{(2\pi\chi)^3(\bar{N}/V)}{(2s+1)\pi^{3/2}(2mkT)^{3/2}} = \mathcal{J}_{1/2}(\alpha_0)$$

α_0 is the chemical potential of the unperturbed system ($e^2 = 0$), i.e., the ideal gas value. The \mathcal{J} functions are

$$\mathcal{J}_m(\alpha) = \frac{1}{\Gamma(m+1)} \int_0^\infty \frac{z^m dz}{1 + \exp(-\alpha + z)} = \sum_{s=1}^m \frac{(-1)^s e^{s\alpha}}{s^{m+1}} \quad \text{for } e^\alpha < 1.$$

Since the chemical potential depends on $\beta\Omega_I$, we write it as $\alpha = \alpha_0 + \delta\alpha$ and now must evaluate $\delta\alpha$ from

$$\bar{N} = \frac{\partial\beta\Omega}{\partial\alpha} = \bar{N} \frac{\mathcal{J}_{1/2}(\alpha_0 + \delta\alpha)}{\zeta} + \frac{\partial\beta\Omega(\alpha_0 + \delta\alpha)}{\partial\alpha}.$$

A Taylor expansion gives

$$\bar{N} = \bar{N} \left\{ 1 + \delta\alpha \frac{\mathcal{J}_{-1/2}(\alpha_0)}{\zeta} + \frac{\delta\alpha^2}{2!} \frac{\mathcal{J}_{-3/2}(\alpha_0)}{\zeta} + \dots \right\} + \frac{\partial\beta\Omega(\alpha_0)}{\partial\alpha_0} + \delta\alpha \frac{\partial^2\beta\Omega(\alpha_0)}{\partial\alpha_0^2} + \dots$$

Clearly when $\beta\Omega_I$ is very small, then $\delta\alpha$ becomes proportional to $\frac{\partial\beta\Omega}{\partial\alpha}$ and higher-order terms may be neglected. Thus the lowest-order result is

$$\delta\alpha = -\frac{\frac{\partial\beta\Omega_I(\alpha_0)}{\partial\alpha}}{\frac{N}{\zeta} \frac{\mathcal{J}_{-1/2}(\alpha_0)}{\partial\alpha_0}} = -\frac{\partial\beta\Omega_I}{\partial N}$$

The second form of $\delta\alpha$ in the above equation follows from

$$dN(\alpha) = \frac{d}{d\alpha} \left[\frac{N}{\zeta} \frac{\mathcal{J}_{-1/2}(\alpha)}{\zeta} \right] d\alpha = \frac{N}{\zeta} \frac{\mathcal{J}_{-1/2}(\alpha)}{\zeta} d\alpha.$$

Also note that to first order in $\delta\alpha$ the following identity holds $\beta\Omega_I(\alpha) = -\beta F_I(\alpha_0)$ where F_I is the interaction free energy (ψ in Siegert's work). Consequently one sees that the quantity $\partial\beta\psi/\partial N$ which appears in the variational derivation of N_z^*, J_z is the first-order shift in the chemical potential away from the ideal-gas value α_0 .

In order to find $\delta\alpha$ more accurately than the above first-order result one must solve at least a quadratic equation. It is possible to do this without too much difficulty for the non-degenerate electron gas. In the limit of no degeneracy all the \mathcal{J} functions reduce to the Boltzmann form, $\mathcal{J}_m(\alpha) = e^\alpha$, and we have

$$\frac{e^\alpha}{\zeta} = \frac{\exp(\alpha_0 + \delta\alpha)}{\zeta} = e^{\delta\alpha}$$

since $e^{\alpha_0} = \zeta$, $\alpha_0 = \log \zeta$.

Classical Coulomb interaction effects in the electron gas are functions of the dimensionless parameter

$$\Lambda = \frac{\beta e^2}{\lambda_D} = \frac{1}{4\pi\rho\lambda_D^3} = 2\pi^{1/2} e^3 \beta^{3/2} \rho^{1/2}, \quad \rho = \frac{N}{V}.$$

In the grand partition function the corresponding quantity is $\Lambda e^{\delta\alpha/2}$ because everywhere N appears it should be replaced with $\bar{N} e^{\delta\alpha}$.

The Helmholtz free energy is

$$\beta F(\rho, \beta) = N \left\{ (\alpha_0 - 1) - \left[\frac{\Lambda}{3} + \frac{\Lambda^2}{12} \left(\log 3\Lambda + 2c - \frac{11}{6} \right) \right] \right\}$$

to order Λ^2 . This includes the Debye-Hückel term and the small Λ form of the Abe S_2 integral. The thermodynamic potential to the same order of accuracy is

$$\beta \Omega(\alpha, \beta) = \bar{N} \left\{ e^{\delta\alpha} + \frac{1}{3} \Lambda \exp\left(\frac{3}{2} \delta\alpha\right) + \frac{\Lambda^2 e^{2\delta\alpha}}{12} \left[\log 3\Lambda \exp\left(\frac{1}{2} \delta\alpha\right) + 2c - \frac{11}{6} + \frac{3}{2} \right] \right\}.$$

Note that $\beta \Omega_I = -\beta F_I$ only to $O(\Lambda)$. To find $\delta\alpha$ one must solve

$$\bar{N} = \frac{\partial \beta \Omega}{\partial \delta\alpha} = \bar{N} \left\{ e^{\delta\alpha} + \frac{1}{2} \Lambda \exp\left(\frac{3}{2} \delta\alpha\right) + \frac{\Lambda^2 e^{2\delta\alpha}}{6} \left[\log 3\Lambda \exp\left(\frac{1}{2} \delta\alpha\right) + 2c - \frac{11}{6} + \frac{3}{2} + \frac{1}{4} \right] \right\}$$

or

$$1 = 1 + \delta\alpha + \frac{1}{2} \delta\alpha^2 + \frac{1}{2} \Lambda \left(1 + \frac{3}{2} \delta\alpha \right) + \frac{\Lambda^2}{6} \left(\log 3\Lambda + 2c - \frac{1}{12} \right).$$

Solving for $\delta\alpha$ to order Λ^2 gives

$$\delta\alpha = -\frac{\Lambda}{2} - \frac{\Lambda^2}{6} \left(\log 3\Lambda + 2c - \frac{19}{12} \right).$$

The above calculation of $\delta\alpha$ was carried out to show how to calculate the chemical potential from the thermodynamic potential obtained as the logarithm of the grand partition function. Now recall from thermodynamics that the chemical potential is the Gibbs' free energy per particle, i.e., $G \equiv E - TS + PV = N\mu$ (our α is $\beta\mu$), and that the chemical potential is obtained from the Helmholtz free energy as $\mu = \frac{\partial F}{\partial N}$. In the case of the classical electron gas we have the result for the Helmholtz free energy (it is easier to calculate than the grand potential in the absence of quantum effects). Carrying out the indicated differentiation gives

$$\delta\alpha = \frac{F_I \frac{\partial \beta}{\partial N}}{\bar{N}} = -\frac{\Lambda}{2} - \frac{\Lambda^2}{6} \left(\log 3\Lambda + 2c - \frac{19}{12} \right)$$

in agreement with the earlier result. One other important result should be noted here. In the absence of degeneracy due to quantum statistics ($\xi \ll 1$ and hence $\omega_0 = \log \xi$ is large and negative) we find, from the defining relation for the number of particles in terms of the grand potential, the expression

$$e^{-\delta\alpha} \equiv \exp\left(-\frac{\partial\beta F_I}{\partial N}\right) = 1 + \frac{\partial\beta\Omega_I}{N e^{\delta\alpha} \partial\alpha} = 1 + \frac{\partial\beta\Omega_I}{\partial N(\alpha)}.$$

Variational Treatment of the Multicomponent Gas (Siegert's Method). We now consider a gas composed of N_i nuclei of charge Z and ZN_i electrons. At sufficiently low temperature this gas will be N_i neutral atoms, and at sufficiently high temperature it will be completely ionized, i.e., N_i bare nuclei and ZN_i free electrons. At intermediate temperatures every ionic species is possible; there will be n_e free electrons and n_z ions of charge z (thus $Z - z$ bound electrons on this ion). These numbers, n_e and n_z , depend on temperature and density, but always must satisfy the requirements

$$\sum_{z=0} n_z = N_i$$

$$\sum_{z=1} zn_z = n_e \text{ (electrical neutrality)}$$

Each ion of charge z may be in one of numerous internal-energy states with quantum numbers which will be denoted collectively as J_z . Of the n_z ions with charge z the number in a state J_z will be denoted as n_{z,J_z} , and thus we have

$$\sum_{J_z} n_{z,J_z} = n_z$$

for z ranging from 0 to $Z - 1$ (ions of charge Z , bare nuclei, of course have no internal states). The energy levels are denoted as $\epsilon(z, J_z, n_e, \{n_z\})$. They are

functions of the number of various kinds of charges because the energy levels of the ion in a vacuum [denoted by $\epsilon^0(z, J_z)$] will be shifted upward due to screening by other charges in the plasma. If one assumes that the least-bound electron on an ion of charge z moves in Coulomb field of charge $z + 1$ (nucleus and core bound electrons) but with this Coulomb field screened according to the Debye prescription, i. e., the effective potential is $-(z + 1)(e^2/r) \exp(-r/\lambda_D)$, then the energy levels will be $\epsilon(z, J_z, n_e, \{n_z\}) = \epsilon^0(z, J_z) + (z + 1)e^2/\lambda_D + \delta\epsilon(J_z, n_e, \{n_z\})$ where the vacuum levels will be hydrogenic, the second term is a constant energy shift upwards for all levels, and the third term will be in lowest approximation

$$\delta\epsilon = -(z + 1) \left(e^2/\lambda_D \right) \langle r/\lambda_D \rangle_{J_z}$$

The assumption has been made here that the energy of the level is measured from the vacuum continuum limit. Actually, however, the continuum limit for electrons is effectively lowered by the amount $-e^2/\lambda_D$. Thus bound levels above this lowered-continuum limit [this means $|\epsilon(z, J_z, n_e, \{n_z\})| < e^2/\lambda_D$] find themselves no longer bound. The number of states to be counted as bound is determined by the condition that $\epsilon(z, J_z, n_e, \{n_z\}) + e^2/\lambda_D = \epsilon^0(z, J_z) + \langle (z + 1)e^2/r - u_{\text{eff}}(r) \rangle_{J_z} + e^2/\lambda_D < 0$. The screened Debye potential is a model for $u_{\text{eff}}(r)$, and not necessarily a good one.

According to basic ideas of statistical mechanics the probability of a given partition of the total energy, i. e., n_e free electrons and the set $\{n_z, J_z\}$ of ions, is

$$W(n_e, \{n_z, J_z\}) = \frac{\left[\frac{(2s_e + 1)V}{\pi^{-3/2} \lambda_e^3} \right]^{n_e} \prod_z \left[\frac{(2s_z + 1)V}{\pi^{-3/2} \lambda_z^3} \right]^{n_z}}{n_e! \prod_z n_z, J_z!} \exp \left\{ -\beta F_I - \beta \sum_{z, J_z} n_z, J_z \epsilon(z, J_z, n_e, \{n_z\}) - \frac{n_0^2 b_2(\beta)}{V} \right\}$$

where $\chi_e = \hbar/(2m_e kT)^{1/2}$, $\chi_i = \hbar/(2m_i kT)^{1/2}$, $b_2(\beta)$ is the second virial coefficient, and n_0 is the number of neutral particles. This expression is essentially Siegert's Eq. (16), (Ref. 4). The first two factors are the translational partition functions of electrons and ions [Siegert did not explicitly put in the translation partition function of ions, i. e., $(V/\chi_i^3)N_i$]. The same thermal wavelength λ_i may be used for each ion because of the smallness of the electron mass compared with ionic masses. s_e and s_i are spins of electrons and ions. In the exponential, F_I is the Coulombic free energy due to interaction of free electrons and ions. In the low density limit, F_I is just the Debye result (ring integral sum for point charges)

$$\beta F_I = -\frac{\beta}{3} \left(n_e + \sum z^2 n_z \right) \frac{e^2}{\lambda_D} = -\frac{1}{3} \frac{V}{4\pi \lambda_D^3}$$

$$\lambda_D = \left[4\pi \beta e^2 \left(\rho_e + \sum z^2 \rho_z \right) \right]^{-1/2}.$$

This result could be improved by treating the ions as extended structures (rather than points) by describing the bound electrons with some kind of form factor. Also it should include the multicomponent form of the Abe S_2 -integral. The terms S_{2ee} and S_{2zz} for electron-electron and ion-ion interaction respectively may be written down immediately in their classical-limit form, but the term S_{2ez} for electron-ion interaction has no classical limit and the correct quantum-mechanical treatment has not yet been dependably evaluated even in the low-density limit. At this point it is not clear how to combine the exact but unevaluated theory with the present elementary approach. The reason is that S_{2ez} includes both scattering states and bound states of electrons on ion of charge z . Bound-state energies, however, are already treated in the second term in the exponential. The third term is the free energy due to interaction among the neutral atoms ($z = 0$), and is approximated with the second virial coefficient.

From this expression for W , we wish to find the most probable partition using the method of Lagrange multipliers. Since we have two conditions to satisfy - fixed

number of nuclei and charge neutrality - we introduce two as yet undetermined multipliers, and calculate the partition for which the quantity

$$\mathcal{L} = \log W + \alpha_i \sum_{z=0}^Z n_z + \alpha_e (n_e - \sum z n_z)$$

is stationary. We now assume that $n_{z,J_z} = n_{z,J_z}^* + \delta n_{z,J_z}$ where the variation $\delta n_{z,J_z}$ must satisfy

$$\sum_{z,J_z} \delta n_{z,J_z} = \sum_z \delta n_z = 0$$

$$\delta n_e = \sum_{z,J_z} z \delta n_{z,J_z} = \sum_z z \delta n_z .$$

Siegert used only one multiplier, α_i , but in his calculation took into account electrical neutrality by replacing δn_e with $\sum z \delta n_z$. The first variation of \mathcal{L} is

$$\begin{aligned} \delta \mathcal{L} = & -\delta n_e \left[\log n_e^* + \log \frac{(2s_e + 1)V}{(\pi^{-1/2} \lambda_e)^3} \right] - \sum \delta n_{z,J_z} \left[\log n_{z,J_z}^* + \log \frac{(2s_z + 1)V}{(\pi^{-1/2} \lambda_1)^3} \right] \\ & - \delta n_e \frac{\partial \beta F_I}{\partial n_e} - \sum_z \frac{\partial \beta F_I}{\partial n_z} \sum_{J_z} \delta n_{z,J_z} - \sum_{z,J} \delta n_{z,J_z} \beta \epsilon(z, J_z, n_e, \{n_z\}) \\ & - \beta \left(\sum_z \frac{\partial \epsilon}{\partial n_e} n_{z,J_z} \right) \delta n_e - \beta \sum_z \left(\sum_{J'_z} n_{z,J'_z} \frac{\partial \epsilon}{\partial n_z} \right) \sum_{J_z} \delta n_{z,J_z} - \frac{2\delta n_0 n_0 b_2}{V} \\ & + \alpha_i \sum \delta n_{z,J_z} + \alpha_e \left(\delta n_e - \sum z \delta n_z \right) = 0 . \end{aligned}$$

Assuming the coefficients of δn_e and $\delta n_{z,J_z}$ to be zero gives

$$\begin{aligned} \log n_{z,J_z}^* &= (\alpha_i - z\alpha_e) + \log \frac{(2s_z + 1)V}{\left(\lambda_1/\pi^{1/2}\right)^3} - \frac{\partial \beta F_I}{\partial n_z} - \beta \epsilon(z, J_z, n_e, \{n_z\}) \\ &\quad - \beta \sum_{J_z} n_{z,J_z}^* \frac{\partial \epsilon}{\partial n_z} - 2\left(\frac{n_0^*}{V}\right) b_2(\beta) \delta_K(z^0) \\ \log n_e^* &= \alpha_e + \log \frac{(2s_e + 1)V}{\left(\lambda_e/\pi^{1/2}\right)^3} - \frac{\partial \beta F_I}{\partial n_e} - \beta \sum_{z,J_z} n_{z,J_z}^* \frac{\partial \epsilon}{\partial n_e}. \end{aligned}$$

The equation for n_{z,J_z}^* contains two terms not present in Siegert's expression: namely, the term containing $\partial \epsilon / \partial n_z$ which takes into account the density dependence of the energy levels and the term involving the second virial coefficient for interaction between neutral atoms. Note that the $\log V$ term can be written as

$$\begin{aligned} \log \frac{(2s_e + 1)V}{\left(\lambda_e/\pi^{1/2}\right)^3} &= \log n_e^* + \log \frac{(2s_e + 1)\pi^{3/2}(2m_e kT)^{3/2}}{(n_e^*/V)^{3/2}} \\ &= \log n_e^* + \log \frac{1}{\zeta_e} = \log n_e^* - \alpha_{e0} \end{aligned}$$

where $\alpha_{e0} = \log \zeta_e$ is the chemical potential in the absence of interaction. Thus, the number of free electrons n_e^* and the occupation numbers, n_{z,J_z}^* , may be written as

$$\begin{aligned} n_e^* &= \frac{(2s_e + 1)\pi^{3/2}V}{\lambda_e^3} \exp \left\{ \alpha_e - \frac{\partial \beta F_I}{\partial n_e} - \beta \sum_{z,J_z} n_{z,J_z}^* \frac{\partial \epsilon}{\partial n_e} \right\} \\ n_{z,J_z}^* &= \frac{(2s_z + 1)\pi^{3/2}V}{\lambda_1^3} \exp \left\{ (\alpha_i - z\alpha_e) - \frac{\partial \beta F_I}{\partial n_z} - \beta \epsilon(z, J_z, n_e, \{n_z\}) \right. \\ &\quad \left. - \beta \sum_{J_z} n_{z,J_z}^* \frac{\partial \epsilon}{\partial n_z} - 2\left(\frac{n_0^*}{V}\right) b_2(\beta) \delta_K(z^0) \right\}. \end{aligned}$$

Our next problem is to determine the undetermined multipliers α_i and α_e . We first need the number of ions of charge z which is

$$n_z^* = \sum_{J_z} n_{z, J_z}^* = \frac{(2s_z + 1)\pi^{3/2}V}{\lambda_i^3} \exp \left\{ (\alpha_i - z\alpha_e) - \frac{\partial \beta F_i}{\partial n_z} \right. \\ \left. - \beta f_z(n_e, \{n_z\}) - \beta \sum_{J_z} n_{z, J_z}^* \frac{\partial \epsilon}{\partial n_z} \right\}$$

where

$$\exp(-\beta f_z) = \sum_{J_z} \exp[-\beta \epsilon(z, J_z, n_e, \{n_z\})].$$

The quantity $\exp(-\beta f_z)$ is the internal partition function of the ion of charge z ; the sum over J_z is to be cut off when the energy levels reach the lowered continuum. Thus, the actual number of levels to be summed in the calculation of the internal free energy, f_z , is probably in most cases a small finite number. Presumably a more accurate theory must take into account the broadening of these bound states near the lowered continuum. The topmost levels may be so broadened that they overlap and thus not contribute as bound states. At the present time, we do not take into account this effect.

Let us look at the occupation number formula, n_{z, J_z}^* , and ask how to recover Siegert's result, Eq. (20), (Ref. 4). First note that Siegert does not have the factor

$$\frac{(2s_z + 1)\pi^{3/2}V}{\lambda_i^3} = N_i(2s_z + 1) \frac{1}{\xi_i} = N_i(2s_z + 1) \exp(-\alpha_{i0})$$

since he left the ion translational partition function out of his W . Secondly, note that his multiplicative factor involving the electron translational partition function may be written as

$$\left(\frac{2V}{\lambda^3 n_e^*} \right)^z = \left(\frac{1}{t_e} \right)^z = \exp(-z\alpha_{e0}) .$$

Thus the exact chemical potential, α_e , in the present result is replaced by the 'ideal gas chemical potential, α_{e0} , in his result. Now note that the formula for n_e^* may be written as

$$1 = \exp \left\{ \alpha_e - \alpha_{e0} - \frac{\partial \beta F_I}{\partial n_e} - \beta \sum_{z, J_z} n_{z, J_z}^* \frac{\partial \epsilon}{\partial n_e} \right\}$$

$$\therefore \alpha_e = \alpha_{e0} + \frac{\partial \beta F_I}{\partial n_e} + \beta \sum_{z, J_z} n_{z, J_z}^* \frac{\partial \epsilon}{\partial n_e} .$$

Actually, Siegert does not lose the piece $\partial \beta F_I / \partial n_e$ that occurs in the exact result for α_e since, in his formula, the partial differentiation, with respect to n_z , must be interpreted as

$$\left(\frac{\partial \beta F_I}{\partial n_z} \right)_{\text{Siegert}} = \frac{\partial \beta F_I}{\partial n_z} + \frac{\partial \beta F_I}{\partial n_e} \frac{\partial n_e}{\partial n_z}$$

where $\partial n_e / \partial n_z = z$ since $n_e = \sum z n_z$. In the present formulas the partial derivatives have the usual meaning, i. e., differentiation only with respect to the stated variable. Thus in the end Siegert has the correct result for n_{z, J_z}^* except for the ion translational partition function. The present method of using two undetermined multipliers seems preferable because it is clear how to do the treatment in the grand partition function, and it is not clear in Siegert's method where only one multiplier, α_I , is used.

Next we must have a procedure to evaluate α_i and α_e . The total number of nuclei N_i is supposed to determine α_i from the equation

$$N_i = \sum_{z=0}^Z n_z^* = \frac{\pi^{3/2} V}{\lambda_i^3} e^{\alpha_i} \left\{ (2s_0 + 1) \exp \left[-\beta f_0 - 2 \left(\frac{n_0^*}{V} \right) b_2(\beta) \right] \right. \\ \left. + \sum_{z=1}^Z (2s_z + 1) \exp \left[-z\alpha_e - \frac{\partial \beta F_I}{\partial n_z} - \beta f_z - \beta \sum_{J_z} n_{z,J_z}^* \frac{\partial \epsilon}{\partial n_z} \right] \right\}.$$

In terms of α_{i0} and α_{e0} the above equation may be written as

$$1 = \exp(\alpha_i - \alpha_{i0}) \sum_{z=0}^Z (2s_z + 1) \exp \left[-z\alpha_{e0} - \frac{\partial \beta F_I}{\partial n_z} - z \frac{\partial \beta F_I}{\partial n_e} - \beta f_z \right. \\ \left. - \beta \sum_{J_z} n_{z,J_z}^* \frac{\partial \epsilon}{\partial n_z} - z\beta \sum_{z,J_z} n_{z,J_z}^* \frac{\partial \epsilon}{\partial n_e} - 2 \left(\frac{n_0^*}{V} \right) b_2 \delta_K(z0) \right].$$

We can calculate $\alpha_i - \alpha_{i0}$ (α_{i0} is known since N_i is a fixed number) as soon as we have α_{e0} ; but α_{e0} depends on the number of free electrons which has yet to be determined. α_e and hence α_{e0} is determined from the electrical neutrality condition, $n_e^* = z n_z^* = \bar{z} N_i$. Here \bar{z} is the average ionic charge which must go to zero at low temperature and to Z at high temperature. The equation for \bar{z} is

$$\bar{z} = \frac{\sum z n_z^*}{\sum n_z^*} = \frac{\sum_{z=1}^Z z (2s_z + 1) \exp \left(-z\alpha_{e0} - \frac{\partial \beta F_I}{\partial n_z} - z \frac{\partial \beta F_I}{\partial n_e} - \beta f_z - \dots \right)}{\sum_{z=0}^Z (2s_z + 1) \exp \left(-z\alpha_{e0} - \dots \right)}$$

where

$$\alpha_{e0} = \log \zeta_e = \log \frac{\pi^3 (\bar{z} N_i / V)}{(2s_e + 1) \pi^{3/2} (2mkT)^{3/2}}.$$

Presumably this equation is solved for \bar{z} by guessing values of \bar{z} , calculating the right-hand side, and repeating until both sides of the equation match. Once α_e and α_i are known we may return to the evaluation of the occupation number formula, \bar{n}_z^*, J_z .

Grand Partition Function Approach to the Multicomponent System. In the grand partition function one allows both the energy and the number of particles to vary in a fixed volume V and at a temperature T . One calculates the average energy and the average number of particles (not the most probable number as in the variational approach). The average number of particles is equated to the actual number in the system and this condition gives an equation for the chemical potential for that type of particle. In our multicomponent gas we have two conditions, fixed number of nuclei N , and electrical neutrality; these conditions will be taken care of by introducing the chemical potentials α_i and α_e exactly as in the variational method. One calculates \bar{N}_i and $\bar{n}_e - \sum z \bar{n}_z$ by differentiating the grand partition function with respect to α_i and α_e respectively. Strictly speaking we cannot get the occupation numbers, \bar{n}_z, J_z , from the grand partition function. However, it turns out that the result for \bar{n}_z is immediately apparent from the result for \bar{N}_i . Furthermore we have ample reason to believe the canonical distribution of energy, and so can write immediately

$$\bar{n}_{z, J_z} = \bar{n}_z \frac{\exp \left[-\beta \epsilon (z, J_z \bar{n}_e \{ \bar{n}_z \}) \right]}{\sum_J e^{-\beta \epsilon_z}} = \bar{n}_z \exp (\beta f_z - \beta \epsilon)$$

Our main problem is the determination of the chemical potentials, and to this end we will derive formula for \bar{N}_i and \bar{z} that are the same as the expressions obtained in the previous section by the variational method.

The grand canonical partition function, assuming classical statistics for all particles, is

$$Z_G(\beta, \alpha_i, \alpha_e) = \sum_{n_e, n_z, J_z} \frac{\exp[\alpha_i \sum n_z + \alpha_e (n_e - \sum z n_z)]}{n_e! \prod n_{z,J_z}!} \prod_z \left[\frac{(2s_z + 1) \pi^{3/2} V}{\lambda_i^3} \right]^{n_z} \left[\frac{(2s_e + 1) \pi^{3/2} V}{\lambda_e^3} \right]^{n_e}$$

$$\times \exp \left[-(\beta F_I)(n_e, \{n_z\}) - \sum n_{z,J_z} \epsilon - \frac{n_0^2 b_2}{V} \right]$$

where the summations over n_e and n_{z,J_z} are unrestricted. In the end, however, α_i and α_e must be chosen so that \bar{N}_i is the actual number of nuclei and the electrical neutrality condition is satisfied, $\bar{n}_e - \sum z \bar{n}_z = 0$. More generally, the summations in the above expression represent the evaluation of the trace of $\exp[\alpha_i \sum n_z + \alpha_e (n_e - \sum z n_z) - \beta H]$. The result for the thermodynamic potential is

$$\beta \Omega = \log Z_G = \bar{n}_e \frac{J_{3/2}(\alpha_e)}{\zeta_e} + \frac{\bar{N}_i}{\zeta_i} \sum_z (2s_z + 1) \exp(\alpha_i - z\alpha_e - \beta f_z) + (\beta \Omega_I) + \frac{n_0^2 b_2}{V}$$

where

$$\zeta_e = \frac{\lambda_e^3 (\bar{n}_e / V)}{(2s_e + 1) \pi^{3/2}} \quad , \quad \zeta_i = \frac{\lambda_i^3 (\bar{N}_i / V)}{\pi^{3/2}}$$

Recall that both Ω_I and f_z are functions of the numbers of particles. This will be expressed as a dependence on the chemical potentials. The prescription is

$$n_z = \bar{N}_i \frac{(2s_z + 1)}{\zeta_i} \exp(\alpha_i - z\alpha_e - \beta f_z)$$

$$n_e = \frac{(2s_e + 1) \pi^{3/2} V}{\lambda_e^3} J_{1/2}(\alpha_e)$$

We are allowing for the possibility that the electrons are sufficiently dense that Fermi statistics causes degeneracy.

The result for \bar{N}_i is

$$\begin{aligned}\bar{N}_i &= \frac{\partial(\beta\Omega)}{\partial\alpha_i} = \left(\frac{V\pi^{3/2}}{\lambda_i^3}\right) e^{\alpha_i} \sum_z (2s_z + 1) \exp(-z\alpha_e - \beta f_z) \left(1 - \beta \frac{\partial f_z}{\partial n_z} n_z\right) \\ &\quad + \sum_z \frac{\partial(\beta\Omega_i)}{\partial n_z} n_z + \frac{2n_0^2 b_2}{V}.\end{aligned}$$

Similarly, differentiation with respect to α_e gives

$$\begin{aligned}\bar{n}_e - \sum_z z\bar{n}_z &= \frac{\partial(\beta\Omega)}{\partial\alpha_e} = \bar{n}_e \frac{\partial 1/2(\alpha_e)}{\partial \zeta_e} + \frac{\partial(\beta\Omega_i)}{\partial n_e} \frac{dn_e}{d\alpha_e} + \bar{N}_i \exp(\alpha_i - \alpha_{i0}) \sum_z (2s_z + 1) \\ &\quad \times \exp(-z\alpha_e - \beta f_z) \left(-z - \beta \frac{\partial f_z}{\partial n_e} \frac{dn_e}{d\alpha_e} + \beta \frac{\partial f_z}{\partial n_z} n_z\right) + \sum_z \frac{\partial(\beta\Omega_i)}{\partial n_z} (-z n_z) = 0.\end{aligned}$$

From these two equations we can pick out the expressions for \bar{n}_z , \bar{n}_e , and $\sum_z z\bar{n}_z$. Our procedure now is roughly the same as in the previous section. The first step is to solve for α_e from the result for \bar{n}_e ; since electron degeneracy is allowed for, this step is more complicated than in the previous section. ζ_e is proportional to the number of free electrons, and consequently the second step is to write down an expression for \bar{z} so that we can calculate the number of free electrons, $\bar{n}_e = \bar{z}\bar{N}_i$. Finally, on knowing α_e we can return to the expression for \bar{N}_i and solve for α_i .

The expression for \bar{n}_e (read from the result for $\bar{n}_e - \sum_z z\bar{n}_z$) is

$$\bar{n}_e = \bar{n}_e \frac{\partial 1/2(\alpha_e)}{\partial \zeta_e} + \frac{\partial(\beta\Omega_i)}{\partial n_e} \frac{\partial n_e}{\partial \alpha_e} - \beta \sum_z \bar{n}_z \frac{\partial f_z}{\partial n_e} \frac{dn_e}{d\alpha_e}$$

or

$$\mathfrak{J}_{1/2}(\alpha_0) = \zeta_e \left[1 + \left(\frac{\partial(\beta\Omega_I)}{\partial n_e} + \beta \sum_z \bar{n}_z \frac{\partial f_z}{\partial n_e} \right) \frac{1}{n_e} \frac{dn_e}{d\alpha_e} \right].$$

This expression defines α_e in terms of ζ_e , but ζ_e is not known until \bar{z} is determined. Recall that

$$\mathfrak{J}_{1/2}(\alpha_e) = e^{\alpha_e} - \frac{e^{\alpha_e}}{2^{3/2}} + \dots$$

Let us solve for e^{α_e} at least to order ζ_e

$$e^{\alpha_e} = \zeta_e + \frac{\zeta_e^2}{2^{3/2}} + \dots$$

$$\begin{aligned} \alpha_e &= \log \zeta_e + \log \left(1 + \frac{\zeta_e}{2^{3/2}} \right) \\ &= \underbrace{\left(\log \zeta_e + \frac{\zeta_e}{2^{3/2}} + \dots \right)}_{\alpha_{e0}} + \left[-\frac{\partial(\beta\Omega_I)}{\partial n_e} + \beta \sum_z \bar{n}_z \frac{\partial f_z}{\partial n_e} \right] \frac{1}{n_e} \frac{dn_e}{d\alpha_e} + \dots \end{aligned}$$

In the limit of no degeneracy (so that the ζ_e term of α_{e0} is negligible compared with $\log \zeta_e$) this expression for α_e is identical to that derived in the previous section.

For the second step of our calculational procedure we need \bar{z} which is

$$\bar{z} = \frac{\sum z \bar{n}_z}{\sum \bar{n}_z} = \frac{\sum_{z=1}^Z z(2s_z + 1) \exp(-z\alpha_e - \beta f_z) \left[1 + \frac{\partial(\beta\Omega_I)}{\partial n_z} - \beta \bar{n}_z \frac{\partial f_z}{\partial n_z} \right]}{\sum_{z=0}^Z (2s_z + 1) \exp(-z\alpha_e - \beta f_z) \left[1 + \frac{\partial(\beta\Omega_I)}{\partial n_z} - \beta \frac{\partial f_z}{\partial n_z} \bar{n}_z + 2 \left(\frac{\bar{n}_0}{V} \right) b_2 \delta_K(z) \right]}.$$

This is the central result of the grand partition function method. As in the result for z in the previous section it may be regarded as an equation for z of the form $\bar{z} = f[\alpha_e(\bar{z})]$, and coupled with the equation defining α_e in terms of \bar{z} it may be solved for any degree of electron degeneracy. It was not clear how to include electron degeneracy in the variational result for z . The next question is: are the two expressions for \bar{z} identical? In the grand partition function result Ω_I appears linearly while in the variational result F_I appears in the exponential. In fact, the two results are the same since it was shown previously that

$$\exp \left[-\frac{\partial \beta F_I(\alpha_0)}{\partial n} \right] = 1 + \frac{\partial \Omega_I(\alpha)}{\partial n(\alpha)} .$$

Finally the third step is to evaluate α_i from the expression for \bar{N}_i which may be written as

$$1 = \exp(\alpha_i - \alpha_{i0}) \sum_{z=0} (2s_z + 1) \exp(-z\alpha_e - \beta f_z) \left[1 + \frac{\partial(\beta\Omega_I)}{\partial n_z} - \beta \frac{\partial f_z}{\partial n_z} n_z + 2\left(\frac{\bar{n}_0}{V}\right)b_2 \right] .$$

Once α_e and α_i are evaluated the number of ions of charge z and the occupation numbers of various states may be found from

$$\bar{n}_z = \bar{N}_i \exp(\alpha_i - \alpha_{i0})(2s_z + 1) \exp(-z\alpha_e - \beta f_z) \left[1 + \frac{\partial(\beta\Omega_I)}{\partial n_z} - \beta \frac{\partial f_z}{\partial n_z} \bar{n}_z \right]$$

$$\bar{n}_{z,J_z} = \bar{n}_z \exp[\beta f_z - \beta \epsilon(z, J_z, \bar{n}_e, \{\bar{n}_z\})] .$$

In order to compare these results with the variational results note also that

$$-\beta \bar{n}_z \frac{\partial f_z}{\partial n_z} = \bar{n}_z \frac{\partial}{\partial n_z} \log \sum_{J_z} e^{-\beta \epsilon} = -\beta \bar{n}_z \frac{\sum \frac{\partial \epsilon}{\partial n_z} e^{-\beta \epsilon}}{\sum e^{-\beta \epsilon}} = -\beta \sum_z \bar{n}_{z,J_z} \frac{\partial \epsilon}{\partial n_z} .$$

Thus, the grand partition function approach reproduces in every respect the results of the variational approach. Also it gives a prescription for inclusion of the effects of electron degeneracy at high density.

Crude Estimation of the Chemical Potential Shifts. Consider again the occupation number formula for a non-degenerate gas as obtained from the variational method

$$\frac{n_{z,J_z}}{N_1} = (2s_z + 1) \exp \left[\alpha_i - \alpha_{10} - z\alpha_{e0} - \beta\epsilon(z, J_z, n_e, \{n_z\}) - \frac{\partial(\beta F_I)}{\partial n_z} - z \frac{\partial(\beta F_I)}{\partial n_e} - \beta n_z \frac{\partial f_z}{\partial n_z} - z\beta n_e \sum_{z'=0}^{z-1} \frac{\partial f_{z'}}{\partial n_e} \right]$$

In the low-density limit βF_I is the Debye result:

$$\beta F_I = \frac{\beta e^2}{3 \lambda_D^2} \left(\sum z^2 n_z + n_e \right), \quad \lambda_D^{-1} = \left[4\pi \beta e^2 \left(\sum z^2 n_z + n_e \right) \right]^{1/2}$$

and the resulting shift in the chemical potentials is found to be

$$\frac{\partial(\beta F_I)}{\partial n_z} + z \frac{\partial(\beta F_I)}{\partial n_e} = \beta(z^2 + z) \frac{e^2}{2\lambda_D^2}.$$

The question now is, how does the shift due to the dependence of the energy levels on charged-particle density compare with the above results? Assume that we have decided how many levels are to go into the calculation of f_z either by taking the last one under the lowered continuum or perhaps the last distinct line before broadening merges the remaining upper levels. Suppose further that we can calculate these levels by solving the Schroedinger equation with the screened Debye potential, $(z + 1)(e^2/r)e^{-r/\lambda_D}$. Suppose further that the resulting energy levels may be

written as an expansion in powers of $(a_0/\lambda_D)/(z + 1)$ since the Bohr radius for the core charge $z + 1$ is $a_0/(z + 1)$

$$\epsilon(z, J_z, n_z, \{n_z\}) = -\frac{(z + 1)^2 Ry}{n^2} + (z + 1) \frac{e^2}{\lambda_D} - a_{1z, J_z} \frac{e^2 a_0}{\lambda_D^2} + a_{2z, J_z} \frac{e^2 a_0^2}{\lambda_D^3} - \dots$$

where the coefficients a_{nz, J_z} are numbers to be calculated from the multipole matrix elements, $\langle r^n/a_0^n \rangle$. Presumably if these energy levels are fed into the calculation of f_z then f_z could also be written as such an expansion

$$f_z = f_z^{(0)} + (z + 1) \frac{e^2}{\lambda_D} - b_{1z} \frac{e^2 a_0}{\lambda_0^2} + b_{2z} \frac{e^2 a_0^2}{\lambda_D^3} - \dots$$

Then the terms in the chemical potential shifts depending on the energy levels would be

$$\begin{aligned} \beta n_z \frac{\partial f_z}{\partial n_z} + z \beta n_e \sum_{z'=0}^{z-1} \frac{\partial f_{z'}}{\partial n_e} &= \frac{\beta e^2}{2\lambda_D} \left\{ \frac{(z + 1)z^2 n_z}{\sum z^2 n_z + n_e} \left[1 - \frac{2b_{1z}}{z + 1} \left(\frac{a_0}{\lambda_D} \right)^2 + \frac{3b_{2z}}{(z + 1)^2} \left(\frac{a_0}{\lambda_D} \right)^2 - \dots \right] \right. \\ &\quad \left. + \frac{zn_e}{\sum z^2 n_z + n_e} \sum_{z'=0}^{z-1} \left[(z' + 1) - 2b_{1z'} \left(\frac{a_0}{\lambda_D} \right) + \frac{3b_{2z'}}{(z' + 1)} \left(\frac{a_0}{\lambda_D} \right)^2 - \dots \right] \right\}. \end{aligned}$$

If the presumed expansion of f_z exists, then we can conclude that at low density, for which $a_0 \ll \lambda_D$, then only the first term of the energy shift should be sufficient, and the above result would be

$$\frac{\beta e^2}{2\lambda_D} \frac{(z + 1)z^2 n_z + zn_e z(z + 1)/2}{\sum z^2 n_z + n_e}.$$

It appears that this result could be of the same order as the shift obtained from the Debye free energy. Certainly the effect should be investigated before much effort is put into using approximations to the Abe S-term to improve the Coulomb free energy.

A. 2 EQUATION OF STATE OF A MULTICOMPONENT PLASMA AT HIGH TEMPERATURE

The purpose of this section is to set forth what is known at present about the free energy of a multicomponent plasma at high temperature and low density. In this limit the Debye-Hückel term with quantum-mechanical diffraction corrections is the dominant Coulomb interaction contribution, namely $O(\rho^{1/2})$. The next term beyond the Debye-Hückel free energy is $O(\rho \log \rho)$, and is the main concern here.

For simplicity, we begin with a discussion of a one-component plasma – the electron gas in a smeared-out positive background to maintain electrical neutrality. In such a plasma there are three fundamental lengths which suffice to describe the system:

$$\text{Distance of closest approach} - l_c = \beta e^2$$

$$\text{Thermal deBroglie wavelength} - \lambda = \hbar(\beta/2m)^{1/2}$$

$$\text{Debye screening length} - \lambda_D = (4\pi\beta e^2\rho)^{-1/2}$$

The three possible ratios of these lengths give the dimensionless parameters which are useful for writing down formulas for the free energy:

$$\text{Classical plasma parameter} - \Lambda = \frac{l_c}{\lambda_D} = \frac{1}{4\pi\rho\lambda_D^3} = 2\pi^{1/2} e^3 \beta^{3/2} \rho^{1/2}$$

$$\text{Quantum diffraction parameter} - \gamma = \frac{\lambda}{\lambda_D} = (2\pi)^{1/2} \hbar e \beta \rho^{1/2} m^{-1/2}$$

$$\text{Wigner-Kirkwood expansion parameter} - \eta = \frac{\lambda}{l_c} = \frac{\gamma}{\Lambda} = 2^{-1/2} \hbar e^{-2} \beta^{-1/2} m^{-1/2}$$

At high temperature the three lengths are ordered as $l_c < \lambda \ll \lambda_D$ and hence the dimensionless parameters satisfy $\Lambda < \gamma < 1$, $\eta > 1$. This is the limit in which we wish to give a correct result for the multicomponent free energy. High temperature here means $kT > Ry$; when this is true then the thermal wavelength is greater than the distance of closest approach, and consequently quantum-mechanical diffraction effects must have some residual importance.

With the work of Meeron and Abe it is now possible to evaluate the free energy of a low-density classical electron gas. The word classical means $\hbar = 0$. Also with the help of the Wigner-Kirkwood expansion one may evaluate small quantum corrections to the classical free energy due to the uncertainty principle. For the Coulomb potential the Wigner-Kirkwood expansion parameter is η as defined above. This parameter becomes large at high temperature, and consequently the WK expansion for the Coulomb potential can only be valid in the low-temperature limit (when $\eta < 1$). This situation contrasts with the WK expansion applied to ordinary non-ideal gases with say a Lennard-Jones interaction where the WK expansion* parameter becomes small at high temperature. The result for the electron-gas free energy in the low-temperature regime is

$$\frac{\beta(F - F_0)}{N} = -\frac{\Lambda}{3} - \frac{\Lambda^2}{12} (\log \Lambda + D_1) \dots + \Lambda^2 f(\eta^2) \quad (A. 1)$$

$$f(\eta^2) = -\frac{\eta^2}{12} + \frac{\eta^4}{60} + \frac{\eta^6}{63} \dots$$

For this result to be valid as written the fundamental lengths are ordered as $\lambda < l_c < \lambda_D$ and the dimensionless parameters as $\gamma < \Lambda < 1$, $\eta < 1$ ($kT < 1$ rydberg). One may ask whether this limit makes any sense because for real electrons Fermi statistics must be considered at low temperatures. We will avoid for the time being any modification due to quantum statistics by the device of giving the electrons a spin s which may be large. The gas remains non-degenerate, i. e., with a nearly Maxwellian velocity distribution as long as $\xi = \rho \lambda^3 / (2s+1) \ll 1$. The gas is partially degenerate when $\xi \sim 1$ and very degenerate when $\xi \gg 1$.

The function $f(\eta^2)$ in Eq. (A. 1) represents the sum of the entire WK series of which only the first three terms have been calculated (and it is unlikely that anymore will ever be evaluated because of the extreme complexity). Obviously this series expansion is only useful when η is small, but in the interesting high-temperature limit we observed that η becomes large. Consequently instead of the WK series

*The WK expansion for various potentials has been discussed by the author:
J. Math. Phys. 3, 1003 (1962).

we must have the asymptotic form of the function $f(\eta^2)$ valid when $\eta \gg 1$. In fact this asymptotic result must be

$$f(\eta^2) \underset{\eta \gg 1}{\sim} \frac{\pi^{1/2}}{2^{7/2}} \eta - \frac{1}{12} \log \eta \dots \quad (A. 2)$$

This asymptotic form used in Eq. (A. 1) gives the high-temperature free energy as

$$\frac{\beta(F - F_0)}{N} = -\frac{\Lambda}{3} \left(1 - \frac{3\pi^{1/2}}{2^{7/2}} \gamma \dots \right) - \frac{\Lambda^2}{12} (\log \gamma + D_2) \dots \quad (A. 3)$$

valid when $\ell_c < \lambda_D \ll \lambda_D$, i.e., $\Lambda < \gamma < 1$ and $\eta > 1$. The asymptotic form of $f(\eta^2)$ as given by Eq. (A. 2) has been arrived at in a round-about fashion, though it is hoped that it will soon be possible to verify it by direct calculation. The diffraction corrections contained in the parentheses multiplying the classical Debye term in Eq. (A. 3) were calculated in an article* by the author, however it was not made clear that the result was valid only when $\gamma > \Lambda$, i.e., when $\eta > 1$. The $\log \gamma$ term in Eq. (A. 3) is the main point of interest.

Simple perturbation theory is helpful in understanding both Eqs. (A. 1) and (A. 3). In first order the direct interaction is

$$1st = \rho_e^2 \int_0^\infty 4\pi r^2 dr \left(-\frac{\beta e^2}{r} \right) \propto -\rho_e^2 (\beta e^2) L^2$$

where L is the length of a side of the container. Thus first-order perturbation theory gives a quadratic divergence, but the term is multiplied by $(\rho_e + z_i \rho_i)$ which must equal zero for electrical neutrality. The second-order term has a linear divergence

$$2nd = \rho_e^2 \int_0^\infty 4\pi r^2 dr \left(-\frac{\beta e^2}{r} \right)^2 \propto \rho_e^2 (\beta e^2)^2 L .$$

*J. Math. Phys. 3, 1216 (1962).

This divergence is removed by summing the ring diagrams which has the effect of introducing Debye screening, so that L in the above expression becomes λ_D . The point is that the familiar Debye-Hückel free energy is really little more than a second-order perturbation result. In third order we have a logarithmic divergence both for long and short distances

$$3rd = \rho_e^2 \int_0^\infty 4\pi r^2 dr \left(-\frac{\beta e^2}{r}\right)^3 \propto \rho_e^2 (\beta e^2)^2 \log \frac{L_{\max}}{l_{\min}}.$$

By summing chains of Coulomb interactions one again introduces Debye screening which has the effect of making L_{\max} into λ_D . The divergence at short distances in the classical gas can be cut off only by summing perturbation theory for two-body interactions to all orders. When this is done the lower cut off l_{\min} becomes the distance of closest approach $l_i = \beta e^2$. These two operations are described nicely by Abe.* Thus one finds the term with $\log \lambda_D/\beta e^2 = -\log \Lambda$ in Eq. (A. 1).

For the high-temperature limit of the electron gas with $\hbar \neq 0$, i.e., $\beta e^2 < \lambda$, the above discussion of simple perturbation theory becomes different in the third order

$$3rd \propto \rho_e^2 (\beta e^2)^2 \log \frac{\lambda_D}{\lambda} \propto -\Lambda^2 \log \gamma$$

and the n th-order term is

$$nth = \rho_e^2 \int_\lambda^\infty 4\pi r^2 dr \left(-\frac{\beta e^2}{r}\right)^n \propto \frac{\rho_e^2 (\beta e^2)^n}{\lambda^{n-3}} \propto \frac{\Lambda^{n-1}}{\gamma^{n-3}}$$

which is negligible compared with third order since we are specifying the high-temperature limit in which $\gamma > \Lambda$. In a certain sense the quantum mechanical result given in Eq. (A. 3) is simpler than the classical result in Eq. (A. 1) because the logarithm in Eq. (A. 3) comes from only third-order perturbation theory while the logarithm in Eq. (A. 1) requires perturbation theory to infinite order.

*Prog. Theo. Phys. 22, 213 (1959).

It should be noted here that the constant D_1 in Eq. (A. 1) is known, namely $D_1 = \log 3 + 2c - 11/6$, while D_2 in Eq. (A. 3) is not known yet.

In addition to Eq. (A. 3) there are also exchange corrections in the high-temperature limit:

$$\frac{1}{2s+1} \left\{ \frac{1}{2} \gamma^2 - \frac{\pi^{1/2} \log 2}{2^{5/2}} \gamma \Lambda + D_3 \Lambda^2 \dots \right\} = \frac{\gamma^2}{2s+1} \left\{ \frac{3}{2} - \frac{\pi^{1/2} \log 2}{2^{5/2}} \frac{\Lambda}{\gamma} + D_3 \left(\frac{\Lambda}{\gamma} \right)^2 \dots \right\} .$$

First-, second-, and third-order exchange interactions are described above. The constant D_3 has not yet been evaluated.

We may now write down the result for the free energy of the multicomponent plasma for high temperature using the previous considerations. In a two-component plasma there is an additional parameter, namely the electron-to-ion mass ratio, m_e/m_i . There will now be three de Broglie wavelengths to be considered, namely for electron-electron interaction, electron-ion interaction, and ion-ion interaction. In a real plasma the ion mass is 2000 times the electron mass or more, and this fact has an interesting effect on the logarithmic term in the free energy. In the temperature region defined by $1 \text{ rydberg} < kT < (m_i/m_e) \text{ rydberg}$, the lengths of the two-component system are ordered as

$$\kappa_{ei} = \pi(\beta/2\mu_{ei})^{1/2}$$

$$\kappa_i < \ell_c < \kappa_{ee} \approx \kappa_{ei} \ll \lambda_D$$

$$\mu_{ei} = m_e m_i / (m_e + m_i)$$

Consequently the cutoffs of the logarithmic divergencies for the electron-electron and the electron-ion interactions are λ_D, κ_{ee} and λ_D, κ_{ei} respectively, while the cut-offs for the ion-ion interaction are like the Abe result in Eq. (A. 1), namely λ_D, ℓ_c . Thus the result for the free energy is

$$\frac{\beta(F - F_0)}{N} = -\frac{\Lambda}{3} - \frac{\Lambda^2}{12} \left\{ f_e^2 \log \frac{\kappa_{ee}}{\lambda_D} - 2z_i^3 f_i \log \frac{\kappa_{ei}}{\lambda_D} + z_i^6 f_i^2 \log \frac{\beta e^2}{\lambda_D} \right\} \quad (A. 4)$$

where $\rho = \rho_e + \rho_i$, $f_e = \rho_e/\rho$, $f_i = \rho_i/\rho$. Here z_i is the charge number of the ion. In Eq. (A.4) diffraction and exchange corrections were not written, because we are looking mainly at the logarithm terms. Note that if the temperature is $kT > (m_i/m_e) Ry$ then the ion-ion interaction term would become $\log \chi_{ii}/\lambda_D$. Also if the electrons and ions have equal and opposite charge and the same mass, the logarithms in Eq. (A.4) would all be equal and the bracket would be multiplied by 0. (This statement applies to ionized positronium!) For real ionized gases, however, the above result depends very much on the electron and ion masses.

This result, Eq. (A.4), is obtainable from simple arguments because the gas at high enough temperature is fully ionized, and further third-order perturbation theory suffices because the thermal wavelength is greater than the distance of closest approach. When these conditions are not fulfilled then the problem is vastly more difficult since the electron-ion interaction includes the possibility of bound states. Thus Eq. (A.4) is probably useful for a hydrogen plasma above say 13 eV. The usefulness of the result is further somewhat limited by the fact that the constant terms D_2 and D_3 for the exchange contribution are not yet known. Nevertheless, Eq. (A.4) as written (and with the known constant D_1) probably gives a good estimate of the free energy down to say about 7 eV.

It is easy to use Eq. (A.4) to obtain a result for the average potential around a particular charge α according to the method described in the next section. The result is

$$\overline{\beta U}_\alpha = z_\alpha \frac{\partial(\beta F)}{\partial z_\alpha} = - \frac{\beta e^2 z_\alpha^2}{\lambda_D} \left[1 + \frac{\Lambda}{2} \left(f_e^2 \log \frac{\chi_{ee}}{\lambda_D} - 2z_i^3 f_e f_i \log \frac{\chi_{ei}}{\lambda_D} + z_i^6 f_i^2 \log \frac{\beta e^2}{\lambda_D} \right) \right]$$

where

$$\Lambda = \frac{1}{4\pi\rho\lambda_D^3}, \quad \rho = \rho_e + \rho_i$$

$$\lambda_D = \left[4\pi\beta e^2 (\rho_e + z_i^2 \rho_i) \right]^{-1/2}.$$

A.3 AVERAGE POTENTIAL AND POTENTIAL FLUCTUATIONS OF A PARTICLE IN A PLASMA

In this section a standard procedure in statistical mechanics is used to derive expressions for the average potential of a particle in an equilibrium plasma and for the root-mean-square fluctuations around the average potential. The method requires only one and two differentiations of the free energy, i. e., the logarithm of the partition function, of the plasma. Thus the results depend entirely on accuracy of the evaluation of the free energy. Explicit results for the average potential and the fluctuations have been obtained for the one-component plasma, i. e., the electron gas, by Bohm and Pines. The end result in this section is a more satisfactory derivation of the Bohm and Pines expression for the potential expression extended to the multicomponent plasma. Since the Debye-Hückel plasma free energy is equivalent to the Bohm-Pines random phase approximation, we know that the resulting expressions for average potential and potential fluctuations are valid in the low-density and high-temperature limit.

Let us first consider the derivation of the total potential energy of a plasma, \bar{U} , and the fluctuation, $\bar{U}^2 - \bar{U}^2$. Our system is a box of volume V containing N_e electrons of charge z_{ee} and N_i ions of charge z_{ie} all at temperature $\beta = 1/kT$. Electrical neutrality requires $z_e N_e + z_i N_i = 0$. The partition function is

$$Z = \exp \{-\beta [F_0 + F_I(g)]\} = \text{Tr} \exp \{-\beta (H_0 + gU)\}$$

$$U = \frac{1}{2} \sum_{j \neq l} \frac{z_e^2 e^2}{r_{jl}} + \sum_{j, \alpha} \frac{z_e z_i e^2}{r_{j\alpha}} + \frac{1}{2} \sum_{\alpha \neq \beta} \frac{z_i^2 e^2}{r_{\alpha\beta}}$$

where g is a dummy dimensionless number which is set equal to 1 at the end, and F_I is the interaction free energy. H_0 is the sum of particle kinetic energies and F_0

is the resulting free energy which gives the ideal gas laws. Differentiation with respect to g gives

$$\frac{\partial(\beta F)}{\partial g} = -\frac{1}{\partial g} \log Z = \frac{\text{Tr} \beta U e^{-\beta H}}{\text{Tr } e^{-\beta H}} = \overline{\beta U}$$

$$\frac{\partial^2(\beta F)}{\partial g^2} = -\frac{\text{Tr}(\beta U)^2 e^{-\beta H}}{\text{Tr } e^{-\beta H}} + \left(\frac{\text{Tr} \beta U e^{-\beta H}}{\text{Tr } e^{-\beta H}} \right)^2 = -\left[(\overline{\beta U})^2 - (\overline{\beta U})^2 \right].$$

The Debye-Hückel plasma free energy with e^2 replaced by ge^2 is $\beta F_I(g) = -1/3 N \Lambda g^{3/2}$ where

$$N = N_e + N_i, \quad \rho = \frac{N}{V}$$

$$\Lambda = \frac{1}{4\pi\rho\lambda_D^3} = 2\pi^{1/2} e^3 \beta^{3/2} \rho^{1/2} \langle z^2 \rangle^{3/2}$$

$$\lambda_D = \left[4\pi\beta e^2 (z_e^2 \rho_e + z_i^2 \rho_i) \right]^{-1/2}$$

$$\langle z^2 \rangle = \frac{(z_e^2 \rho_e + z_i^2 \rho_i)}{\rho}$$

Differentiating this free-energy expression with respect to g gives

$$\overline{\beta U} = -\frac{1}{2} N \Lambda$$

$$(\overline{\beta U})^2 - (\overline{\beta U})^2 = +\frac{1}{4} N \Lambda.$$

The plasma interaction parameter Λ may be rewritten as

$$\Lambda = \frac{\beta e^2 \langle z^2 \rangle}{\lambda_D} = 4\pi e^4 \beta^2 \rho \lambda_D^2 \langle z^2 \rangle^2$$

and consequently the potential energy and the fluctuation become

$$\bar{U} = - \frac{N}{2} \left(\frac{\beta e^2}{\lambda_D} \right) \langle z^2 \rangle$$

$$\overline{U^2} - \bar{U}^2 = \frac{1}{4} N 4\pi e^4 \lambda_D \rho \langle z^2 \rangle^2$$

where the fluctuation has been written in a form similar to the Bohm-Pines results.

The average energy of any single particle in the plasma and its fluctuation is obtained in a similar manner. If the potential energy is

$$U = \frac{1}{2} \sum_{j \neq \ell} \frac{z_j z_\ell e^2}{r_{j\ell}}$$

where the indices j and ℓ run over every particle in the plasma, electrons and protons, then statistical averages are obtained by differentiating with respect to the charge number z_α of particle α . Thus, we find

$$\frac{\partial(\beta F)}{\partial z_\alpha} = \frac{\text{Tr} \beta \sum_j \frac{z_j e^2}{r_{\alpha j}} e^{-\beta H}}{\text{Tr} e^{-\beta H}} = \frac{1}{z_\alpha} \left(\overline{\beta \sum_j \frac{z_\alpha z_j e^2}{r_{\alpha j}}} \right) = \frac{\overline{\beta U_\alpha}}{z_\alpha}$$

$$\frac{\partial^2(\beta F)}{\partial z_\alpha^2} = - \frac{\text{Tr} \beta^2 \left(\sum_j \frac{z_j e^2}{r_{\alpha j}} \right)^2 e^{-\beta H}}{\text{Tr} e^{-\beta H}} + \left[\frac{\text{Tr} \beta \left(\sum_j \frac{z_j e^2}{r_{\alpha j}} \right) e^{-\beta H}}{\text{Tr} e^{-\beta H}} \right]^2 = - \overline{(\beta U_\alpha)^2} - \overline{(\beta U_\alpha)^2}$$

Similarly

$$\frac{\partial^2(\beta F)}{\partial z_\alpha \partial z_{\alpha'}} = - \left[\left(\overline{\beta^2 U_\alpha U_{\alpha'}} \right) - (\overline{\beta U_\alpha})(\overline{\beta U_{\alpha'}}) \right].$$

If the Debye-Hückel free energy is written as

$$\beta F_I = - \frac{1}{3} 2\pi^{1/2} e^3 \beta^{3/2} V^{-1/2} \left(\sum z_j^2 \right)^{3/2}.$$

Then the indicated differentiations are easily carried out to obtain

$$\frac{\overline{\beta U_\alpha}}{z_\alpha} = - (2\pi^{1/2} e^3 \beta^{3/2} V^{-1/2}) z_\alpha \left(\sum_j z_j^2 \right)^{1/2}$$

or

$$\overline{\beta U_\alpha} = - N \Lambda \frac{z_\alpha^2}{\sum_j z_j^2} = - \frac{\beta e^2 z_\alpha^2}{\lambda_D}.$$

This is an important result. It says that a particle of charge $z_\alpha e$ even with no kinetic energy has a negative potential energy amounting to $(z_\alpha e)^2 / \lambda_D$. For an electron ($z_e = -1$) this is the amount by which the continuum is effectively lowered, i.e., bound electrons in an atom are effectively unbound when the binding energy is less than e^2 / λ_D . The particle α feels a potential $\overline{\phi}_\alpha$ defined by $\overline{U}_\alpha = (z_\alpha e) \overline{\phi}_\alpha$ which is $\overline{\phi}_\alpha = - z_\alpha e / \lambda_D$. Note that this is not a constant potential for each particle. Both $\overline{\phi}_\alpha$ and \overline{U}_α depend on the charge $z_\alpha e$ because the potential and resulting potential energy are caused by a polarization of the plasma in the neighborhood of α . Thus like charges are repelled and unlike charges attracted.

If we sum \overline{U}_α over all α we get twice the actual total potential energy of the plasma because each interacting pair of particles is counted twice. Thus, $\sum \overline{U}_\alpha = 2\overline{U}$. Our expressions for \overline{U}_α and \overline{U} satisfy this requirement.

Similarly the fluctuation in U_α is

$$\begin{aligned} \overline{(\beta U_\alpha)^2} - \overline{(\beta U_\alpha)}^2 &= -z_\alpha^2 \frac{\partial^2 F_I}{\partial z_\alpha^2} = z_\alpha^2 (2\pi^{1/2} e^{3/2} \beta^{3/2} V^{-1/2}) \left[\left(\sum z_j^2 \right)^{1/2} + \frac{z_\alpha^2}{\left(\sum z_j^2 \right)^{2/3}} \right] \\ &= N\Lambda \left[\frac{z_\alpha^2}{\left(\sum z_j^2 \right)^2} + \frac{z_\alpha^4}{\left(\sum z_j^2 \right)^2} \right] = \Lambda \left[\frac{z_\alpha^2}{\langle z^2 \rangle} + \frac{z_\alpha^4}{N \langle z^2 \rangle^2} \right]. \end{aligned}$$

The first term of this result is of order N^0 and hence interesting; the second term is of order $1/N$ and hence negligible. For completeness, however, one should note that the correlation between U_α and $U_{\alpha'}$ (α and α' being different particles) is

$$\beta^2 \overline{U_\alpha U_{\alpha'}} - \beta^2 \overline{U_\alpha} \overline{U_{\alpha'}} = -z_\alpha z_{\alpha'} \frac{\partial^2 F_I}{\partial z_\alpha \partial z_{\alpha'}} = N\Lambda \frac{z_\alpha^2 z_{\alpha'}^2}{\left(\sum z_j^2 \right)^2} = \Lambda \frac{z_\alpha^2 z_{\alpha'}^2}{N \langle z^2 \rangle^2}.$$

Finally to establish a relation between the fluctuation in U_α and the fluctuation in U , we note that

$$\begin{aligned} \sum_\alpha \left[\overline{(\beta U_\alpha)^2} - \overline{(\beta U_\alpha)}^2 \right] + 2 \sum_{\alpha \neq \alpha'} \left[\overline{\beta^2 U_\alpha U_{\alpha'}} - \overline{\beta^2 U_\alpha} \overline{U_{\alpha'}} \right] &= N\Lambda \left[\frac{\sum z_\alpha^2}{\sum z_j^2} + \frac{\left(\sum z_\alpha^2 \right)^2}{\left(\sum z_j^2 \right)^2} \right] \\ &= 2N\Lambda = 8 \left[\overline{(\beta U)^2} - \overline{(\beta U)}^2 \right] \end{aligned}$$

which is correct since the relation between the fluctuation in \bar{U} and U_α is

$$\frac{1}{2} \sum_{\alpha \neq \alpha'} \left(\overline{U_\alpha U_{\alpha'}} - \overline{U_\alpha} \overline{U_{\alpha'}} \right) = 4 \left(\overline{U^2} - \overline{U}^2 \right).$$

If we ignore the term of order $1/N$, the fluctuation in U_α may be written as $\overline{U_\alpha^2} - \overline{U_\alpha}^2 = 4\pi e^4 \lambda_D \rho \langle z^2 \rangle z_\alpha^2 = 4\pi z_\alpha^2 e^4 \lambda_D (z_e^2 \rho_e + z_i^2 \rho_i)$. This expression is the correct multicomponent generalization of the Bohm-Pines result for the fluctuation. It is valid for high temperature and low density since it was derived from the Debye-Hückel result for the free energy which in turn is valid when $\Lambda \ll 1$. It may be improved by including in the free energy the next-order term which is the multicomponent form of the Abe S_2 -integral. For point electrons and ions the classical form of S_2 is divergent, and consequently a quantum-mechanical treatment is required. Although the correct quantum form of S_2 has yet to be evaluated exactly, it seems clear that at low density ($\Lambda \ll 1$) that the limiting form is of the order $\Lambda^2 \log \Lambda$. For the one-component gas for which the correct form of S_2 is known (since it is classical) one may estimate quite well the error in neglecting S_2 for small values of Λ . It seems that the expressions for U_α and $\overline{U_\alpha^2} - \overline{U_\alpha}^2$ should be correct to a few percent for $\Lambda \lesssim 0.3$.

It should be noted that the fluctuation in U_α becomes arbitrarily large in the limit of high temperature since λ_D goes to ∞ as $(kT)^{1/2}$. Physically this means that the potential felt by any one particle in the plasma changes violently as other plasma particles pass by at high velocities. As we go to lower temperatures and higher densities two effects will begin to change the previous results for $\overline{U_\alpha}$ and $\overline{U_\alpha^2} - \overline{U_\alpha}^2$. First, the electrons begin to be slightly degenerate because they obey Fermi statistics. This means that low-energy electrons cannot so easily change their energy state, and thus contribute less to the screening effect. The ions may always be treated according to classical Boltzmann statistics because of their large mass. Secondly, the electrons are no longer strictly points but are wave packets with extension of roughly the thermal deBroglie wavelength, $\kappa = \hbar/(2mkT)^{1/2}$. The interaction of the wave packets causes quantum-mechanical diffraction effects in the free energy which are of the order of $\Lambda\gamma$ where $\gamma = \lambda/\lambda_D$. As we will now show both effects tend to reduce $\overline{U_\alpha}$ and $\overline{U_\alpha^2} - \overline{U_\alpha}^2$ from our previous results (the particle α is now an electron). The Debye-Hückel free energy for a multicomponent plasma with lowest order corrections for Fermi statistics and wave mechanics is

$$\beta F_I = -\frac{N}{12\pi\rho\lambda_s^3} \left\{ 1 - \frac{\pi^{3/2}}{2^{7/2}} \left(\frac{m_e}{m_i} \right) \frac{\kappa}{\lambda_s} \dots \right\}$$

where

$$\lambda_s = \left(\frac{kT}{4\pi e^2 \beta \rho \langle z^2 \rangle} \right)^{1/2}$$

$$\langle z^2 \rangle = \frac{(z_e^2 \theta_e^2 N_e + z_i^2 N_i)}{N_i}$$

$$\theta_e^2 = \frac{J_{-1/2}(\alpha)}{J_{1/2}(\alpha)} = \frac{\partial N(\alpha)/\partial \alpha}{N(\alpha)} ; \quad N(\alpha) = (2s+1) \int \frac{d^3 p}{(2\pi\hbar)^3} \frac{1}{1 + \exp(-\alpha + \beta p^2/2m)}$$

$$A\left(\frac{m_e}{m_i}\right) = \frac{\left\{ z_e^4 N_e^2 + 2z_e^2 z_i^2 N_e N_i \left(\frac{1 + m_e/m_i}{2} \right)^{1/2} + z_i^4 N_i^2 \right\}}{\langle z^2 \rangle^2}.$$

The quantity θ_e is a measure of the extent to which degenerate electrons are frozen at the bottom of the Fermi distribution and prevented from taking part in the screening. Thus the effective electronic charge for screening changes from e to $\theta_e e$. At high temperature θ_e goes to 1 (the Maxwell-Boltzmann value), and as $T \rightarrow 0$ then θ_e also goes to 0. If we now carry out the differentiation of βF_I with respect to the charge of one electron, then the results for \bar{U}_α and $\bar{U}_\alpha^2 - \bar{U}_\alpha^2$ are

$$\bar{U}_\alpha = - \frac{e^2 \theta_e^2}{\lambda_s} \left\{ 1 - \frac{4}{3} \frac{\pi^{3/2}}{2^{7/2}} A \gamma_e \dots \right\}$$

$$\bar{U}_\alpha^2 - \bar{U}_\alpha^2 = 4\pi \theta_e^2 e^4 \lambda_s \rho \langle z^2 \rangle \left\{ 1 - \frac{4}{3} \frac{\pi^{3/2}}{2^{7/2}} A \gamma_e \dots \right\}.$$

Thus electron degeneracy reduces the results by the factor θ_e^2 , and wave-mechanical diffraction by the multiplicative factor in the braces. Of these two effects diffraction is certainly the more important near the classical limit. To see this fact one notes that generally γ_e is greater than Λ . The statistics factor θ_e^2 is approximately equal to $1 - \xi/2^{3/2}$ where

$$\xi_e = \frac{(2\pi\hbar)^3 \rho_e}{(2s+1)(2\pi m_e kT)^{3/2}} \propto \frac{\gamma_e^3}{\Lambda}.$$

Thus even though ξ_e may be very small (hence very little degeneracy), the diffraction correction may still be significant.

Consider now any solid material with, say, nuclear charge Z . If the material is compressed then the outermost least-bound electrons are squeezed into the continuum. In ordinary metals at room temperature this pressure ionization has already occurred without compression, i.e., each metal atom has lost on the average one electron which circulates freely through the metal. Since solid densities are assumed the electron gas is very degenerate; this means that $kT \ll \epsilon_F$ where ϵ_F is the Fermi energy. Furthermore since the ions are bound in a lattice at all stages of compression (unless the temperature is hot enough to melt the lattice), we have a one-component plasma of electrons with nearly stationary ions forming the neutralizing positive background. The free energy of such an electron gas is known to be

$$F = N_e \left(\frac{p_F^2}{2m} \right) \left\{ \frac{3}{5} - \frac{3}{8} \left[\varphi - \frac{1}{3} (1 - \log 2) \varphi^2 \log \varphi + B\varphi^2 + C\varphi^3 \log \varphi + \dots \right] \right\}$$

\uparrow \uparrow \uparrow
 Ideal gas First-order exchange Gell-Mann and Brueckner
 correlation energy

where

$$\varphi = \frac{4}{\pi} \frac{me^2}{\hbar p_F} = \lim_{T \rightarrow 0} \frac{\gamma^2}{\alpha} \frac{2\alpha^{1/2}}{\pi^{1/2} \xi}$$

$$\alpha = \frac{\mu}{kT} \rightarrow \frac{\epsilon_F}{kT} \text{ as } T \rightarrow 0$$

$$\xi = \frac{(2\pi\hbar)^3 \rho}{2(2\pi mkT)^{3/2}}$$

$$\gamma = \frac{\lambda}{\lambda_D}$$

Hence

$$\varphi = \varphi \left(\frac{\sum z_j^2}{N_e} \right)$$

since electronic charge is $z_j = 1$. This expansion in φ is valid at high density. In terms of the usual parameter $r_s = r_0/a_0$ where $\rho^{-1} = (4\pi/3)r_0^3$ and $a_0 = \hbar^2/me^2$, the expansion is thought to be valid for $r_s < 1$ ($\varphi \sim 0.7r$). In ordinary metals r_s ranges from 2 to 5. Assuming that our material is compressed sufficiently that $r_s < 1$ for the free electrons, one sees that the first-order exchange energy is the dominant contribution to the potential energy. In what follows we consider this to be the case. The average potential felt by any one electron is easily found to be

$$\begin{aligned} \bar{U}_\alpha &= z_\alpha \frac{\partial F}{\partial z_\alpha} \Bigg|_{z_\alpha=1} = z_\alpha \frac{\partial F}{\partial \varphi} \frac{\partial \varphi}{\partial z_\alpha} \Bigg|_{z_\alpha=1} \\ &= -\frac{3}{4} \epsilon_F \varphi \left\{ 1 - \frac{2}{3} (1 - \log 2) \varphi \log \varphi + \left[2B - \frac{1}{3} (1 - \log 2) \right] \varphi + \dots \right\} = -\frac{3}{4} \varphi \epsilon_F \end{aligned}$$

when $\varphi \ll 1$.

$$\bar{U}_\alpha = -\frac{3}{4} \frac{4}{\pi} \frac{me^2}{\hbar p_F} \frac{p_F^2}{2m} = -\frac{3}{2\pi} \frac{e^2 p_F}{\hbar} .$$

Since

$$p_F = \left(\frac{9\pi}{4} \right)^{1/3} \frac{\hbar}{r_0}$$

we have

$$\begin{aligned} \bar{U}_\alpha &= -\frac{3}{2\pi} \left(\frac{9\pi}{4} \right)^{1/3} \frac{e^2}{r_0} = -\frac{3(3\pi^2)^{1/3}}{2\pi} e^2 \rho_e^{1/3} \\ &= -1.48 e^2 \rho_e^{1/3} . \end{aligned}$$

This result is extremely similar to the result from the ion-sphere theory even to the numerical coefficient. Presumably bound electrons will go into the continuum when their binding energy is less than the magnitude of U . The last electron is bound with an energy of $-Z^2$ rydbergs. So presumably the material becomes completely pressure ionized when $\bar{U}_\alpha = -Z^2$ Ry or $1.48 e^2 (ZN_i/V)^{1/3} = Z^2 13.6$ eV, $(N_i/V)^{1/3} = Z^{5/3} 0.55 \times 10^{+8}$ cm⁻¹. Hence a nuclear spacing of $\ell_i = (N_i/V)^{-1/3} = 1.82 \times 10^{-8} Z^{-5/3}$ cm. In terms of r_s for electrons this means $r_s = 2.03/Z^2$. Thus hydrogen becomes a metal at a density of $N_i/N = (0.55 \times 10^{-8})^3 = 0.166 \times 10^{24}$ (atoms cm⁻³).

Appendix B COMPUTER CODE MULTIPLET

A brief description of the code MULTIPLET and the usage thereof is contained in this appendix. Input-output information is provided in Sec. B. 1. Section B. 2 lists the FORTRAN parameters used by the code, their definitions, and their dimensions. Section B. 3 provides a brief description of each subroutine of the code, and a list of the complete source program constitutes Sec. B. 4.

B. 1 INPUT-OUTPUT

A. Data Cards are read in the following order (FORTRAN FORMAT in parentheses).

1. Card 1 - NTAG, (I 10): NTAG = 0, Generate LINE ATLAS and calculate Planck mean.

NTAG = 1, Calculate Planck mean from previously calculated LINE ATLAS on Tape Unit A5.

NTAG = 2, Rosseland calculation (see Appendix D.)

2. Card 2 - (Included only if NTAG = 0).

NCASE, (I 10): Number of atomic data cards

ALPHA0, (E 10. 8): Minimum occupation α_0 .

3. Card 3 - NCASE Atomic Data Cards - (Included only if NTAG = 0). One card per atomic state:

i, (I2)
 γ , (I2)
n, (I2)
 ℓ , (I1)
2S + 1, (I1)
L, (I1)

} Identification of atomic state
(see end of Sec. 2).

β , (I1): **Temperature index**
 E , (E10.8): **Energy of the atomic state in eV relative to the ground state of the neutral atom of the species**
ALPHA(J), (6E8.6): Occupation numbers of the state at the six densities ($J = 1, 6$)
4. Card 4 - ABSMIN, (E20.8): Factor for minimum line strength accumulated in tabulated absorption coefficients
TEMP, (E20.8): Temperature (eV)
NENGY, (I10): Number of different tables of the accumulated absorption coefficient
5. Card 5 - DENS (1, J), (6E12.6): Ion densities (particles/cm³) at the 6 densities ($J = 1, 6$)
6. Card 6 - DENS (2, J), (6E12.6): Electron densities (particles/cm³) at the 6 densities ($J = 1, 6$)
7. Cards 7 - 15 - PSI2, (8F5.4)
PSI1, (17F4.1)
PSI, (17F4.4)
(8 cards) } Data for Voigt profile (listed in Sec. B. 4)
8. NENGY Energy spectrum cards - One card for each table of the accumulated absorption coefficient
NOMEGA, (I10): $N_{\omega} \leq 2000$
OMEGA0, (E20.8): ω_0
DOMEGA, (E20.8): $\Delta\omega$ } (see end of Sec. 4)
B. The systems input tape is Tape 5; the systems output tape is Tape 6. Tapes 16 (=A6) and 25 (=B5) are used as scratch tapes for storage of intermediate results.

Tape 26 (=B6) contains tables of atomic data necessary for the LINE ATLAS calculation (in three files).

First file. HFS radial integrals σ^2 in three tables:

ASLATE ($28 \times 36 \times 2$)

BSLATE ($28 \times 7 \times 36$)

CSLATE (24×36)

Second file. Hydrogenic f-numbers in two tables:

A ($8 \times 8 \times 16$)

B ($8 \times 8 \times 16$)

Third file.

- Shell-averaged hydrogenic f-numbers:

FSHELL (8, 8)

- Series-limit information for line broadening calculation:

SERLIM ($11 \times 12 \times 2$)

Tape 15 (=A5) contains the final results of the calculation: the LINE ATLAS and the table of the accumulated absorption coefficients for broad lines at each of the six densities - NENCY tables, one for each card $[N_\omega, \omega_0, \Delta\omega]$ read. The arrangement of these data on the tape follows.

First File. The LINE ATLAS

- First Record - LTOT: Total number of lines in LINE ATLAS.

NCASE: See Data Card 2

ALPHA0: See Data Card 2

IBETA: Temperature index

- For each of the LTOT lines there is one record (written by subroutine ATLAS).

DELTAE: ΔE = energy (in eV) of line center

Z: the angular factor $\mathcal{A}M$ (see Sec. 4)

FNO:	The f-number
SIGSQ:	σ^2 [see Eq. (4.6)]
GFACT:	The statistical factor G_{ij} of Sec. 4
WCOLL:	Collision width per electron, $[w_j/\rho_e (\text{cm}^{-3})]$ of Eq. (4.11)
WDOPP:	Doppler width $\delta/2$ of Eq. (4.12)
ID1I:	$(100i + \gamma)$
ID2I:	$[1000n + 100\ell + 10(2S + 1) + L]$
	($i \gamma n \ell S L$) of the initial atomic state (see end of Sec. 2)
EI:	energy (in eV) of the initial atomic state
ID1F } ID2F }	Identification of the final atomic state
ALPHA:	Six occupation numbers of the initial atomic state at the six densities being treated.
XMCSQ:	Mass of the atom in eV

Second File.

- First Record - NENCY: The number of absorption coefficient tables

- NENCY tables of the absorption coefficient (each table consisting of seven records):

Record 1 - NOMEGA }
 OMEGA0 }
 DOMEWA }
 OMEGA (2000 words) the energies
 $\epsilon_N = \omega_0 + (N - 1) \Delta\omega, (N = 1, N_\omega)$

Six records of 2000 words each (one for each density J) containing ABS (N, J), the absorption coefficient (cm^{-1}) at energy ϵ_N due to broad lines (N = 1, 2000)

C. The Output Listing

1. The atomic data cards (A-3) (if NTAG = 0), arranged in order of increasing energy (written by MAIN PROGRAM)
2. The LINE ATLAS (if NTAG = 0)

Two lines printed per transition:

First line (see B) - ΔE , FNO, σ^2 , WCOLL, WDOPP, ID (initial state), Energy (initial state), ID (final state), Energy (final state)

Second line - the absorption coefficient (cm^{-1}) at the line center (assuming a Lorentz profile) for each unmerged line at each of the six densities for which the occupation of the initial state is greater than α_0 (written by subroutine ATLAS)

3. The narrow line contribution to the Planck mean at the six densities (written by subroutine ABS)
4. The line absorption coefficient (cm^{-1}) due to broad lines for the six densities at the energies $\epsilon_N = \omega_0 + (N - 1)\Delta\omega$, ($N = 1, N_\omega$) (written by subroutine TALLY)
5. The broad line contribution to the Planck mean opacity at the six densities (written by subroutine MEAN)

Note items 3, 4, and 5 are repeated NENGY times, once for each portion of the energy spectrum designated by a NENGY card.

B. 2 DEFINITIONS OF PARAMETERS IN COMMON STORAGE

Dimensions of dimensioned variables are given in parentheses.

A. MULTIPLET I

J1	0 for oxygen, 1 nitrogen	$\left. \begin{matrix} i \\ \gamma \\ n \\ l \\ 2S + 1 \\ L \end{matrix} \right\}$	Decomposed initial state ID
J2	charge state		
J3			
J4			
J5			
J6			
J7			

J1P	{	1	{	Decomposed final state ID
J2P				
J3P	{	γ'		
J4P				
J5P	{	n'		
J6P				
J7P	{	l'		

IBETA	β = temperature index
NCASE	Number of initial states (≤ 1500)
ALPHA0	α_0 = minimum occupation treated
ALPHA	(1500×6) $\alpha(I, J)$ = occupation of state I at density J
E	(1500) $E(I)$ = energy of state I
ID1	(1500) { ID of atomic state I
ID2	(1500) }
B	(1500×3) Working storage
NREC	Number of tape records on scratch tapes
LTOT	Total number of line transitions
NTOT	
NDIM	NDIM = 1590

B. MULTIPLET II AND III

ABSMIN	Factor defining minimum value of absorption coefficient to be tallied (taken as 0.0001)
TEMP	kT in eV
NENGY	Number of tables of the absorption coefficient
DENS	(2×6) : $DENS(1, J)$ = number ions/cm ³ at density J $DENS(2, J)$ = number electrons/cm ³ at density J
NSLIM	(6) : $NSLIM(J)$ = series limit $n_m(J)$ at density J
NMAX	Largest of $NSLIM(J)$
WFACT	Width factor = $0.637 \times 10^{-22} (kT)^{-1/2}$

LTOT	Number of lines in LINE ATLAS	
K1	i	
K2		
IGI	γ_i	
NI	n_i	
LI	l_i	
KSI	$(2S_i + 1)$	
LAI	L_i	
NSI	n_{si} = number 2s-electrons	
NPI	n_{pi} = number 2p-electrons	
L12I	$(L_{12})_i$ = orbital angular momentum of core	
IS12I	$(2S_{12} + 1)_i$ = core spin-multiplicity	
IGF	γ_f	
NF	n_f	
LF	l_f	
KSF	$(2S_f + 1)$	
LAF	L_f	
NSF	n_{sf} = number 2s-electrons	
NPF	n_{pf} = number 2p-electrons	
L12F	$(L_{12})_f$ = orbital angular momentum of core	
IS12F	$(2S_{12} + 1)_f$ = core spin-multiplicity	
DELTAE	$\Delta\epsilon = \hbar\omega$ = energy of line center in eV	
Z	Angular result	
ALPHA	(6): $\alpha(J)$ = fractional occupation of state at density J	
FNO	f - number of transition	
SIGSQ	σ^2 = square of radial integral of transition	
GFACT	Statistical factor of transition	
WCOLL	Collision width per free electron for transition	
WDOPP	Doppler width for transition	
EI	Energy of initial atomic state (eV)	
XMCSQ	Mass of ion in eV (Mc^2)	

DENMIN Smallest electron density > 0

C. MULTIPLET II:

ASLATE	$(28 \times 36 \times 2)$	Tables of Hartree-Fock-Slater radial integrals σ^2 (see description of subroutine SLATER)
BSLATE	$(28 \times 7 \times 36)$	
CSLATE	(24×36)	
A	$(8 \times 8 \times 16)$:	$A(n, l + 1, n')$ = hydrogenic $f(n, l \rightarrow n', l + 1)$
B	$(8 \times 8 \times 16)$:	$B(n, l + 1, n')$ = hydrogenic $f(n, l \rightarrow n', l - 1)$
FSHELL	(8×8) :	FSHELL $(n' - 8, n - 8)$ = shell-averaged hydrogenic f number $f(n \rightarrow n')$, $n = 9 - 16$, $n' = 9 - 16$
SERLIM	$(11, 12, 2)$:	SERLIM $(J, \gamma, 1)$ = series limit (eV) of configuration $J = 6K_1 + K_2$, γ = core label SERLIM $(J, \gamma, 2)$ = effective quantum number for shell-averaged width evaluation

D. MULTIPLET III

NOMEGA	N_{ω} (≤ 2000) = number energies in one absorption coefficient table
OMEGA0	ω_0 : } Define the energy table OMEGA (in eV)
DOMEGA	$\Delta\omega$: }
OMEGA	(2000): The photon energies at which the absorption coefficient is tabulated: $\text{OMEGA}(N) = \omega_0 + (N-1)\Delta\omega$, ($N = 1, N_{\omega}$)
ABS	(2000 \times 6): $\text{ABS}(N, J) = \text{absorption coefficient (cm}^{-1}\text{)}$ due to broad lines at energy N , density J
AB	(6): Working storage
PSI 1	(17)
PSI 2	(8)
PSI	(17 \times 8) } Data for Voigt profile (Input Cards 6-15) Listed in Sec. B.4

B. 3 THE MULTIPLET FORMULA SET

Note subroutines special to nitrogen and oxygen - or atoms isoelectronic thereto - are indicated by an asterisk.

A. MAIN PROGRAM (Utilizes COMMON and DIMENSION of MULTIPLET I.)

1. If NTAG = 0 - Reads and lists atomic data cards. Calls MULTIPLET I (the subroutines LINE, ORDER, TWRITE) to determine all allowed radiative transitions between the specified atomic states and calculate the angular integrals thereof. The resulting transition data are then written onto a scratch tape in order of increasing photon energy, and program proceeds to MULTIPLET II.

If NTAG = 1 - A previously generated LINE ATLAS is on Tape Unit A5.
Calls MULTIPLET III.

2. Calls MULTIPLET II (the subroutines MSET, ATLAS) to calculate the f-numbers for the transitions determined by MULTIPLET I and generate the LINE ATLAS.
3. Calls MULTIPLET III (the subroutines ABS, FINIS) to evaluate from the LINE ATLAS the broad line absorption coefficient and to calculate the Planck mean opacity.

B. MULTIPLET I

1. ENSORT - Arranges data from atomic data cards in order of increasing energy
2. LINE - For each pair of states specified by the atomic data cards, decomposes the ID's and calls COP to apply selection rules and calculate angular factors if allowed transition. Resulting transitions arranged in order of increasing photon energy by BSORT.

*2.1 COP - Applies selection rules to a given pair of atomic states to determine allowed transitions, calculates angular integral Z.

*2.1.1 O - Determines number of electrons in the 2s-shell of a given atomic state.

*2.1.2 P - Determines number of electrons in the 2p-shell of a given atomic state.

*2.1.3 Q2 - Determines L_{12} = orbital angular momentum of the core for a given atomic state.

*2.1.4 S2 - Determines S_2 = total spin of the 2p-shell for a given atomic state.

*2.1.5 S12 - Determines S_{12} = total spin of the core for a given atomic state.

*2.1.6 FPC - Determines fractional parentage coefficient for decoupling a 2p-electron from a given atomic state.

2.1.7 U - Calculates Jahn coefficient.

2.1.7.1 W - Calculates Racah coefficient.

2.1.7.1.1 SF - $SF(A, B) = B!/(A - 1)!$

2.2 BSORT - Arranges data in data array B in order of increasing energy.

3 ORDER - Arranges transitions in order of increasing photon energy.

3.1 LIST - Writes ordered transitions onto Tape B5 (2000 transitions per record).

3.2 ASORT - Arranges data in data array ALPHA in order of increasing energy.

4 TWRITE - Transfers ordered transitions from Tape B5 to Tape A6 - one transition per record.

C. MULTIPLET II

1 MSET - Reads density cards, calculates merging limit [Eq. (4.13)], and calls TREAD to read Tape B6.

*1.1 TREAD - Reads tables of atomic data from Tape B6.

*2 ATLAS - For each transition on Tape A6, the f-number, collision width, and Doppler width are evaluated by subroutines FCALC and WIDTH. The resulting LINE ATLAS is written onto Tape A5 and is listed.

*2.1 FCALC - The f-number is evaluated for a given transition - according to the prescriptions of Sec. 2.

*2.1.1 SLATER - For a given transition the HFS values of the radial integral are determined from tables ASLATE, BSLATE, CSLATE, as follows:

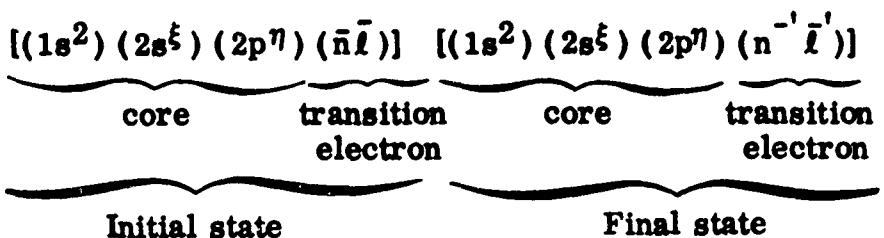
Species index $x_1 = (0, 1)$, charge state x_2

Initial state $[(1s^2)(2s^x)(2p^y)(n^l^z)]$

Final state $[(1s^2)(2s^{x'})(2p^{y'})(n'^{l'}^{z'})]$

(a) $(n, l) \neq (n', l')$ or $(n, l) = (n', l') = 0$

Arrange transition electron into fourth position:



The core is now the same for the initial and final states

Core index $C = 12\xi + 6x_1 + x_2$ ($1 \leq C \leq 36$)

If $\bar{n} = \bar{n}'$: $\sigma^2 = \text{ASLATE}(k, C, s)$

$$k = 7\bar{l} + (\bar{n}-1), s = (3 + \bar{l}' - \bar{l})/2$$

If $\bar{n} \neq \bar{n}'$: If necessary, interchange initial and final states such that $\bar{l}' = \bar{l} - 1$

$$\sigma^2 = \text{BSLATE}(\bar{n} - 1, \bar{n}' - 1, C)$$

(b) $(n, l) = (n', l) \neq 0$: transition is a 2s - 2p transition in the presence of a passive (n, l) electron ($n \geq 3$)

$$\sigma^2 = \text{CSLATE } (6l + n - 2, 12x + 6x_1 + x_2)$$

*2.1.2 FHYDRO - For a given transition determines the hydrogenic f-numbers from Tables A, B.

*2.2 WIDTH - Calculates the Doppler and collision widths, the effective quantum number ν being determined with the use of Table SERLIM.

D. MULTIPLET III:

1 ABS - For each table of the absorption coefficient (NENGY tables in all): transitions are read from the LINE ATLAS one at a time. If the line is a narrow line its contribution to the Planck mean is accumulated. If the line is a broad line, its line center is shifted to the nearest mesh point and the line intensity is evaluated over the photon energy spectrum OMEGA - following each line tail until the resulting intensity is less than ABSMIN times the previously accumulated intensity. Calls TALLY. Lists narrow line contribution to the Planck mean.

1.1 VOIGT - Determines Voigt line profile using Tables PSI1, PSI2, PSI, and limiting series expansions. If $W_{DOPP} < 0.2 W_{COLL}$ or $(\epsilon - \epsilon_c) > 5 W_{DOPP}$ the approximation is

$$b(\epsilon) = \frac{W_c}{2\pi} \left[\frac{1}{(\epsilon - \epsilon_c + 0.7071W_{DOPP})^2 + W_c^2} \right. \\ \left. + \frac{1}{(\epsilon - \epsilon_c - 0.7071W_{DOPP})^2 + W_c^2} \right]$$

1.2 TALLY - Absorption coefficient table written onto Tape B5 and listed

2 FINIS - Transfers absorption coefficient tables from Tape B5 to second file of Tape A5. Calls MEAN.

2.1 MEAN - Evaluates and lists the broad line contribution to the Planck mean - by numerical integration of the tabulated absorption coefficient for each of the NENCY tables.

B.4 LIST OF SOURCE PROGRAM OF MULTIPLET

2	25	3333	50	66671	2	5	25	30	35	40	45	50	PSI1	1
0	2	4	6	8	10	12	14	16	18	20	25	30	PSI1	2
98119797975496849587946593209153896887678552797073556736613655715048	PSI1	3												
97136692962995269385920990028768851282387950720064475731507444873970	PSI1	4												
9519948593859222900387348425808371873396953600251264360371131712724	PSI1	5												
90548995882185448179745726467576241573524541563287262021617341441	PSI1	6												
8550847082357865738868366244564305745063999295722121692132610630869	PSI1	7												
75797470715866756071540147184063346429362486196211580845064305050408	PSI1	8												
5456533149744413806314525221979153211810916051803290230017001320106	PSI1	9												
2868277825252156173613230960067104570309021009500550038002800210017	PSI1	10												

```

C      MULTIPLET (PLANK) MAIN PROGRAM
*
      COMMON J1,J2,J3,J4,J5,J6,J7,J1P,J2P,J3P,J4P,J5P,J6P,J7P,IBETA,
1     NCASE,ALPHAO,ALPHA0,E, ID1, ID2, B,NREC, LTOT, NTOT,NDIM
      DIMENSION ALPHA(1500,6),E(1500),ID1(1500),ID2(1500),B(1500,3)
      REWIND 15
      REWIND 16
      REWIND 25
      REWIND 26
      NDIM=1500
      READ INPUT TAPE 5, 1000, NTAG
      IF (NTAG) 10, 10, 200
10    READ INPUT TAPE 5, 1010, NCASE, ALPHAO
      IF (NCASE-NDIM) 50, 50, 20
      20  WRITE OUTPUT TAPE 6, 1015, NCASE
      CALL EXIT
      50 IF (NCASE-1) 60, 60, 70
      60 WRITE OUTPUT TAPE 6, 1020, NCASE
      CALL EXIT
      70 READ INPUT TAPE 5, 1025, (ID1(I), ID2(I), IBETA, E(I), (ALPHA(I,J),
1     J=1,6), I=1,NCASE)
      CALL ENSORT(NCASE)
      C  WRITE INPUT DATA
      80 LC=100
      DO 100 K=1,NCASE
      100 IF (LC-50) 90, 90, 85
      85 WRITE OUTPUT TAPE 6, 1030, NCASE, ALPHAO,IBETA
      LC=1
      90 WRITE OUTPUT TAPE 6, 1040, K, ID1(K), ID2(K), E(K), (ALPHA(K,J)),
1     J=1,6)
      LC=LC+1
100  CONTINUE
      CALL LINE
      CALL ORDER
      CALL TWRITE
      REWIND 25
      MULT 10
      MULT 20
      MULT 30
      MULT 40
      MULT 50
      MULT 60
      MULT 70
      MULT 80
      MULT 90
      MULT 100
      MULT 110
      MULT 120
      MULT 130
      MULT 140
      MULT 150
      MULT 160
      MULT 170
      MULT 180
      MULT 190
      MULT 200
      MULT 210
      MULT 220
      MULT 230
      MULT 240
      MULT 250
      MULT 260
      MULT 270
      MULT 280
      MULT 290
      MULT 300
      MULT 310

```

```

REWIND 15
200 CALL MSET
IF (INTAG) 210,210,300
210 CALL ATLAS
300 CALL ABS
400 CALL FINIS
401 CALL UNLOAD(26)
CALL EXIT
1000 FORMAT(110)
1010 FORMAT(110,E10.8)
1015 FORMAT(16H1 TOO MANY STATES,110)
1020 FORMAT(15H1 TOO FEW STATES,110)
1025 FORMAT(14,15,11,E10.8,6E8.6)
1030 FORMAT(28H1MULTIPL ET DATA LIST- NCASE=14,13H
1      4X,6H BETA=14/114HO 1
2HA(1)   ALPHA(2)   ALPHA(3)
3A(6)///)
1040 FORMAT(15,115,15,1P7E13.5,/)
END

```

```

*   FORTRAN
*   SUBROUTINE ENSORT(NEN)
C   ARRANGE INITIAL STATES INTO ORDER OF INCREASING ENERGY-
COMMON J1,J2,J3,J4,J5,J6,J7,J1P,J2P,J3P,J4P,J5P,J6P,J7P,IBETA,
1 NCASE,ALPHAO,ALPHA, E, ID1, ID2, B,NREC, LTOT, NTOT,NDIM
DIMENSION ALPHA(1500,6),E(1500),ID1(1500),ID2(1500),B(1500,3)
NE=NEN-1
DO 100 I=1,NE
NEP=I+1
DO 100 J=NEP,NEN
IF(E(I)-E(J)) 100, 100, 20
20 Y=E(I)
E(I)=E(J)
E(J)=Y
Y=ID1(I)
ID1(I)=ID1(J)
ID1(J)=Y
Y=ID2(I)
ID2(I)=ID2(J)
ID2(J)=Y
DO 30 K=1,6
Y=ALPHA(I,K)
ALPHA(I,K)=ALPHA(J,K)
30 ALPHA(J,K)=Y
100 CONTINUE
RETURN
END
EN SORT 0
EN SORTC1
MP C1
MP C2
MP D1
EN SORT 1
EN SORT 2
EN SORT 3
EN SORT 4
EN SORT 5
EN SORT 6
EN SORT 7
EN SORT 8
EN SORT 9
EN SORT10
EN SORT11
EN SORT12
EN SORT13
EN SORT14
EN SORT15
EN SORT16
EN SORT17
EN SORT18
EN SORT19
EN SORT20
EN SORT +

```

```

* FORTRAN
* SUBROUTINE LINE
COMMON J1,J2,J3,J4,J5,J6,J7,J1P,J2P,J3P,J4P,J5P,J6P,J7P,IBETA,
1 NCASE,ALPHAO,ALPHA, E, ID1, ID2, B, NREC, LTOT, NTOT,NDIM
DIMENSION ALPHA(1500,6),E(1500),ID1(1500),ID2(1500),B(1500,3),
L=0
NREC=0
LTOT=0
DO 10 N=1,NDIM
10 B(N,1)=100000.
REWIND 15
REWIND 16
N=NCASE-1
DO 110 I=1,N
DO 115 J=1,6
115 IF(ALPHA(I,J)-ALPHA0) 15,20,20
15 CONTINUE
GO TO 110
20 J1=ID1(I)/1000
J2=(ID1(I)-1000*J1)/100
J3=ID1(I)-1000*J1-100*J2
J4=ID2(I)/1000
J5=(ID2(I)-1000*J4)/100
J6=(ID2(I)-1000*J4-100*J5)/10
J7=ID2(I)-1000*J4-100*J5-10*J6
NP=I+1
DO 100 K=NP, NCASE
100 J1P=ID1(K)/1000
J2P=(ID1(K)-1000*J1P)/100
J3P=ID1(K)-1000*J1P-100*J2P
J4P=ID2(K)/1000
J5P=(ID2(K)-1000*J4P)/100
J6P=(ID2(K)-1000*J4P-100*J5P)/10
J7P=ID2(K)-1000*J4P-100*J5P-10*J6P
40 CALL COP(SW,Z)
40 IF(SW-15.0) 100,50,100

```

```

50 L=L+1
      LTOT=LTOT+1
      IF(LTOT-1000000) 70,70,60
60  WRITE OUTPUT TAPE 6, 1000
      CALL EXIT
70  B(L,1)=E(K)-E(I)
      B(L,2)=Z
      B(L,3)=2000.0*FLOATF(K)+FLOATF(I)
      IF(L-NDIM)100,80,80
80  WRITE TAPE 15,8
90  NREC=NREC+1
      L=0
      DO 95 LP=1,NDIM
95  B(LP,1)=1000000.0
100  CONTINUE
110  CONTINUE
      REWIND 15
120  CALL BSORT(L)
      RETURN
1000 FORMAT(47HNUMBER TRANSITIONS EXCEEDS 100,000. CALL EXIT-)
      END

```

```

*   FORTRAN THIS IS SUBROUTINE COP. IN THIS ROUTINE
*   Z IS COMPUTED.
*   SUBROUTINE COP(SW,Z)
COMMON J1,J2,J3,J4,J5,J6,J7,J1P,J2P,
1J3P,J4P,J5P,J6P,J7P
1F(J4-1)200,200,1
1 IF(J4P-1)200,200,2
2 Z=1.
A1=0(J1,J2,J3,J4,J5,J6,J7)
A1P=0(J1P,J2P,J3P,J4P,J5P,J6P,J7P)
A2=P(J1,J2,J3,J4,J5,J6,J7)
A2P=P(J1P,J2P,J3P,J4P,J5P,J6P,J7P)
A3=A3P=0.0
A4=A5, AND A4P=A5P
A4=Q2(J1,J2,J3,J4,J5,J6,J7)
A5=A4
A4P=Q2(J1P,J2P,J3P,J4P,J5P,J6P,J7P)
A5P=A4P
A7=S2(J1,J2,J3,J4,J5,J6,J7)
A8=S12(J1,J2,J3,J4,J5,J6,J7)
A6=ABSF(A7-A8)
A7P=S2(J1P,J2P,J3P,J4P,J5P,J6P,J7P)
A8P=S12(J1P,J2P,J3P,J4P,J5P,J6P,J7P)
A6P=ABSF(A7P-A8P)
IF(J1-J1P)200,201,200
200 SW=0.
RETURN
201 IF(J2-J2P)200,202,200
202 IF(J4-3)2031,2031,100
2031 IF(J4P-3)203,203,300
203 IF(J7-9)205,204,205
204 IF(J6-J6P)200,300,200
205 IF(J7P-9)206,204,206
206 IF(J7-J7P)207,204,207
207 IF(XABSF(J7-J7P)-1)200,204,200

```

C
C

```

00000010
00000020
00000030
00000040
00000050
00000060
00000070
00000080
00000090
00000100
00000110
00000120
00000130
00000140
00000150
00000160
00000170
00000180
00000190
00000200
00000210
00000220
00000230
00000240
00000250
00000260
00000270
00000280
00000290
00000300
00000310
00000320
00000330
00000340
00000350

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```

300 IF(J4-2)400,301,400
301 IF(J4P-2)700,302,700
302 IF(A1-A1P-1.0)200,500,200
500 Z=Z*A1*(A2+1.0)*FPC(A2P,A7,A4,A4P)*(2.*A5P+1.0)*
1(2.*A8+1.0)
A=.5
B=J6
B=(B-1.0)/2.
Z=Z*U(A,A6P,A7,B,A6,A7P)**2
IF(Z)600,200,600
600 SW=15.
600 RETURN
700 IF(J4P-3)1300,701,1300
701 IF(A1-A1P)704,702,704
702 IF(A2-A2P-1.0)200,703,200
703 IF(J5P)1000,900,1000
704 IF(A1-A1P-1.0)200,705,200
705 IF(A2-A2P)200,706,200
706 IF(J5P-1)200,800,200
800 IF(A5-A5P)200,801,200
801 A=J7P
B=J6
A=2.*A+1.
C=.5
D=(B-1.0)/2.
Z=Z*A1*A*B*U(C,A6P,D,A7,A6,A8P)**2
IF(Z)600,200,600
900 A=J7
A=2.*A+1.
B=J6
C=.5
D=(B-1.0)/2.
Z=Z*A2*FPC(A2,A7P,A4)*A*B*U(C,A7P,D,A6,A7,
1A9P)**2
IF(Z)600,200,600
950 A=J7

```

```

00C000360
00000370
00000380
00000390
00000400
00000410
00000420
00000430
00000440
00000450
00000460
00000470
00000480
00000490
00000500
00000510
00000520
00000530
00000540
00000550
00000560
00000570
00000580
00000590
00000600
00000610
00000620
00000630
00000640
00000650
00000660
00000670
00000680
00000690
00000700
00000710

```

```

A=2.*A+1.
B=J6
C=.5
D=(B-1.)/2.
Z=Z+A2*A*B*U(C,A7P,D,A6,A7,A8P)**2
1F(Z)600,200,600
1F(J5P-2)200,1001,200
1F(J7P-9)1100,1200,1100
1100 A=J7
A=2.*A+1.
B=J6
C=.5
D=(B-1.)/2.
Z=Z+10.*A2*FPC(A2,A7P,A4P,A7,A4)**A*B*U(C,A7P,D,A6,A7,
1A8P)**2
A=J7
B=1.
C=2.
D=J7P
Z=Z*U(A,B,A4P,C,D,B)**2
1F(Z)1600,200,600
1200 A=J7
A=2.*A+1.
B=J6
C=.5
D=(B-1.)/2.
Z=Z+10.*A2*FPC(A2,A7P,A4P,A7,A4)**A*B*U(C,A7P,D,A6,A7,
1A8P)**2
1F(Z)1600,200,600
1300 IF(J4P-9) 1350, 200, 200
1350 IF(A1-A1P)1304,1301,1304
1301 IF(A2-A2P-1)1200,1302,200
1302 IF(J5P)1303,950,1303
1303 IF(J5P-2)200,1200,200
1304 IF(A1-A1P-1)200,1305,200
1305 IF(A2-A2P)200,1306,200
00000720
00000730
00000740
00000750
00000760
00000770
00000780
00000790
00000800
00000810
00000820
00000830
00000840
00000850
00000860
00000870
00000880
00000890
00000900
00000910
00000920
00000930
00000940
00000950
00000960
00000970
00000980
00000990
00001000
00001010
00001020
00001030
00001040
00001050
00001060
00001070

```

1800 A=J7
 1F121600,200,600
 2*2*A*8
 B=J6
 2
 A=2,*A+1.
 1700 A=J7
 1F12)600,200,600
 2
 B=J6
 A=2.*A+1.
 1600 A=J7P
 00001340
 00001330
 00001320
 00001310
 00001300
 00001290
 00001280
 00001270
 00001260
 00001250
 00001240
 00001230
 00001220
 00001210
 00001200
 00001190
 00001180
 00001170
 00001160
 00001150
 00001140
 00001130
 00001120
 00001110
 00001100
 00001090
 00001080
 1306 1F12)600,200,600
 1500 1F1A5-A5P1200,1501,200
 1501 A=J7
 A=2.*A+1.
 B=J6
 C=5
 D=18-1/2.
 E=2*3.*A1*A8*B#UIC,A6P,D,A7,A6,A8P1##2
 400 1F12)600,200,600
 401 1F13-33P1404,402,404
 402 1F15)409,403,409
 403 1F15P-11200,405,200
 404 1F1A1-A1P-1,1200,406,200
 405 1F1A2P-A2-1,1200,407,200
 406 1F1A8-A8P1200,407,200
 407 1F1A5-A5P1408,2200,408
 408 1F1A85P1A5-A5P1-1,200,2200,200
 410 1F15P-11200,412,200
 411 1F15-21200,411,200
 412 1F15-912000,2100,2000
 413 1F15P)414,1700,414
 414 1F15P-21200,415,200
 415 1F17P-911800,1900,1800
 416 1F15P
 417 1F15P-11200,416,200
 418 1F15P-11200,417,200
 419 1F15P-11200,418,200
 420 1F15P-11200,419,200
 421 1F15P-11200,420,200
 422 1F15P-11200,421,200
 423 1F15P-11200,422,200
 424 1F15P-11200,423,200
 425 1F15P-11200,424,200
 426 1F15P-11200,425,200
 427 1F15P-11200,426,200
 428 1F15P-11200,427,200
 429 1F15P-11200,428,200
 430 1F15P-11200,429,200
 431 1F15P-11200,430,200
 432 1F15P-11200,431,200
 433 1F15P-11200,432,200
 434 1F15P-11200,433,200
 435 1F15P-11200,434,200
 436 1F15P-11200,435,200
 437 1F15P-11200,436,200
 438 1F15P-11200,437,200
 439 1F15P-11200,438,200
 440 1F15P-11200,439,200
 441 1F15P-11200,440,200
 442 1F15P-11200,441,200
 443 1F15P-11200,442,200
 444 1F15P-11200,443,200
 445 1F15P-11200,444,200
 446 1F15P-11200,445,200
 447 1F15P-11200,446,200
 448 1F15P-11200,447,200
 449 1F15P-11200,448,200
 450 1F15P-11200,449,200
 451 1F15P-11200,450,200
 452 1F15P-11200,451,200
 453 1F15P-11200,452,200
 454 1F15P-11200,453,200
 455 1F15P-11200,454,200
 456 1F15P-11200,455,200
 457 1F15P-11200,456,200
 458 1F15P-11200,457,200
 459 1F15P-11200,458,200
 460 1F15P-11200,459,200
 461 1F15P-11200,460,200
 462 1F15P-11200,461,200
 463 1F15P-11200,462,200
 464 1F15P-11200,463,200
 465 1F15P-11200,464,200
 466 1F15P-11200,465,200
 467 1F15P-11200,466,200
 468 1F15P-11200,467,200
 469 1F15P-11200,468,200
 470 1F15P-11200,469,200
 471 1F15P-11200,470,200
 472 1F15P-11200,471,200
 473 1F15P-11200,472,200
 474 1F15P-11200,473,200
 475 1F15P-11200,474,200
 476 1F15P-11200,475,200
 477 1F15P-11200,476,200
 478 1F15P-11200,477,200
 479 1F15P-11200,478,200
 480 1F15P-11200,479,200
 481 1F15P-11200,480,200
 482 1F15P-11200,481,200
 483 1F15P-11200,482,200
 484 1F15P-11200,483,200
 485 1F15P-11200,484,200
 486 1F15P-11200,485,200
 487 1F15P-11200,486,200
 488 1F15P-11200,487,200
 489 1F15P-11200,488,200
 490 1F15P-11200,489,200
 491 1F15P-11200,490,200
 492 1F15P-11200,491,200
 493 1F15P-11200,492,200
 494 1F15P-11200,493,200
 495 1F15P-11200,494,200
 496 1F15P-11200,495,200
 497 1F15P-11200,496,200
 498 1F15P-11200,497,200
 499 1F15P-11200,498,200
 500 1F15P-11200,499,200
 501 1F15P-11200,500,200

```

B=2.*A+1.
C=J6
Z=Z*10.*B*C
B=1.
C=2.
D=J7P
Z=Z*U(A,B,A4,C,D,B)**2
IF(Z)1600,200,600
1900 Z=10.
GO TO 1700
2000 A=J7
B=2.*A+1.
C=J6
Z=Z*6.*B*C
B=1.
C=J7P
D=2.
Z=Z*U(A,B,A4,B,C,D)**2
IF(Z)1600,200,600
2100 Z=10.
GO TO 1600
2200 IF(J5-J5P)200,2201,200
2201 IF(J5-212300,2202,2300
2202 IF(J7-912203,2204,2203
2203 IF(J7P-912300,2400,2300
2204 IF(J7P-912500,2600,2500
2300 A=J7P
B=2.*A+1.
C=J6
Z=Z*A1*(A2+1.)*B*C
B=J5
C=1.
D=J7
E=5
Z=Z*U(A4,B,C,A,D,A4P)**2*FPC(A2P,A7,A4,A7P,A4P)
1*U(E,A6P,A7,A8,A6,A7P)**2
00001440
00001450
00001460
00001470
00001480
00001490
00001500
00001510
00001520
00001530
00001540
00001550
00001560
00001570
00001580
00001590
00001600
00001610
00001620
00001630
00001640
00001650
00001660
00001670
00001680
00001690
00001700
00001710
00001720
00001730
00001740
00001750
00001760
00001770
00001780
00001790

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```

2400 IF(Z)600,200,600
      A=J7
      A=2.*A+1.
      B=J6
      C=.5
      Z=Z*A1*(A2+1.)*(2.*A4P+1.)*A*B/(2.*A4+1.)*
      1U(C,A6P,A7,A8,A6,A7P)**2*FPC(A2P,A7,A4,A7P,A4P)
      1F(Z)600,200,600
2500 A=J7P
      A=2.*A+1.
      B=J6
      C=.5
      Z=Z*A1*(A2+1.)*A*B*U(C,A6P,A7,A8,A6,A7P)**2*
      1FPC(A2P,A7,A4,A7P,A4P)
      1F(Z)600,200,600
2600 A=J6
      B=.5
      Z=Z*5.*A1*(A2+1.)*(2.*A4P+1.)*A*U(B,A6P,A7,A8,A6,
      1A7P)**2*FPC(A2P,A7,A4,A7P,A4P)
      1F(Z)600,200,600
2700 IF(J4P-3)200,2750,2750
      IF(J4P-9)2701,200,200
2701 IF(J3-J3P)1200,2702,200
2702 IF(J5)12704,2703,2704
2703 IF(J5P-1)200,2800,200
2704 IF(J5-1)310,2705,310
2705 IF(J5P)2706,1700,2706
2706 IF(J5P-2)200,3000,200
2800 Z=3.
      GO TO 1700
3000 Z=10.
      GO TO 1700
310 1F(J5-2)200,311,200
311 1F(J5P-1)313,312,313
312 1F(J7-9)330,320,330
313 1F(J5P-3)200,314,200
00001800
00001810
00001820
00001830
00001840
00001850
00001860
00001870
00001880
00001890
00001900
00001910
00001920
00001930
00001940
00001950
00001960
00001970
00001980
00001990
00002000
00002010
00002020
00002030
00002040
00002050
00002060
00002070
00002080
00002090
00002100
00002110
00002120
00002130
00002140
00002150

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```

314 IF(J7-7)340,350,340
320 A=J6
Z=30.*((2.*A4+1.)*A
      IF(Z)600,200,600
330 Z=6.
GC TO 1700
340 Z=21.
GO TO 1700
350 A=J6
Z=105.*((2.*A4+1.)*A
      IF(Z)600,200,600
100 IF(J3-J3P)101,385,101
101 IF(J4-J4P)200,102,200
102 IF(J4-9)108,103,103
103 IF(A1-A1P-1.)1200,104,200
104 IF(A2P-A2-1.)1200,105,200
105 IF(A8-A8P)200,106,200
106 IF(A5-A5P)107,380,107
107 IF(ABS((A5-A5P)-1.)200,380,200
108 IF(J5-J5P)200,109,200
109 IF(A1-A1P-1.)200,110,200
110 IF(A2P-A2-1.)200,111,200
111 IF(A8-A8P)200,112,200
112 IF(A5-A5P)113,114,113
113 IF(ABS((A5-A5P)-1.)200,114,200
114 IF(J5-4)360,115,115
115 IF(J5-4)200,370,200
360 A=.5
B=J5
B=2.*B+1.
Z=2.*A1*((A2+1.)*(2.*A4P+1.)*(2.*A8+1.)*
      1FPC(A2P,A7,A4,A7P,A4P)*U(A,A6P,A7,A8,A6,A7P)**2*
28
370 IF(Z)600,200,600
      A=.5
      B=J4

```

```

Z=2.*A1*(A2+1.)*(2.*A4P+1.)*(2.*A8+1.)*
1IFPC(A2P,A7,A4,A7P,A4P)*U(A,A6P,A8,A6,A7P)**2*
2*(B*B-16.*0)
1IF(Z)600,200,600

380 A=.5
B=J4
Z=2.*A1*(A2+1.)*(2.*A4P+1.)*(2.*A8+1.)*B*B*
1IFPC(A2P,A7,A4,A7P,A4P)*U(A,A6P,A8,A6,A7P)**2
1IF(Z)600,200,600
00002520
00002530
00002540
00002550
00002560
00002570
00002580
00002590
00002600
00002610
00002620
00002630
00002640
00002650
00002660
00002670
00002680
00002690
00002700
00002710
00002720
00002730
00002740
00002750
00002760
00002770
00002780
00002800
00002810
00002820
00002830
00002840
00002850
00002860

385 1IF(J4P-16)390,390,200
390 1IF(J4P-J4)200,391,391
391 1IF(J4-4)395,392,395
392 1IF(J4P-9)393,440,440
393 1IF(J5P-J5+1)394,430,394
394 1IF(J5P-J5-1)200,420,200
395 1IF(J4-8)397,397,396
396 Z=-3.
GO TO 600
00002690
00002700
00002710
00002720
00002730
00002740
00002750
00002760
00002770
00002780
00002800
00002810
00002820
00002830
00002840
00002850
00002860

397 1IF(J4P-8)398,398,3101
398 1IF(J5-4)393,399,399
399 1IF(J5-J5P)200,3100,200
3100 1IF(J5-4)200,42,200
3101 1IF(J5-4)3102,399,3102
3102 1IF(J5-4)440,200,200
42 Z=-2.
GO TO 600
00002750
00002760
00002770
00002780
00002790
00002800
00002810
00002820
00002830
00002840
00002850
00002860

430 A=J5
Z=2.*A*(4.*A*A-1.)*(2.*A5+1.)*(2.*A8+1.)*
1IF(Z)600,200,600
420 A=J5P
Z=2.*A*(4.*A*A-1.)*(2.*A5+1.)*(2.*A8+1.)*
1IF(Z)600,200,600
END

```

```

*      FORTRAN
*      FUNCTION O(I1,I2,I3,I4,I5,I6,I7)
C      COMPUTES NUMBER OF ELECTRONS IN THE 2S SHELL
I=I1+I2
IG=I3
      GO TO (8,9,10,11,12,13),I
      8  GO TO (3,3,2,2,2,1),IG
      9  GO TO (3,3,3,2,2,2,1,1),IG
      10 GO TO (3,2,2,2,2,1,1,1),IG
      11 GO TO (3,2,2,1,1,1),IG
      12 GO TO (2,1),IG
      13 IF (I4-2)14,14,1
      14 IL=I+17
      GO TO (2,1),IL
      12 IF (I4+IG+I7-3)3,3,16
      1  O=0
      1  O=0
      1  RETURN
      2  O=1
      2  RETURN
      3  O=2
      3  RETURN
      END

```

```

*      FORTRAN
*      FUNCTION P(I1,I2,I3,I4,I5,I6,I7)
C      COMPUTES NUMBER OF ELECTRONS IN THE 2P SHELL
      I1=I3
      I=I1+I2
      GO TO 10,9,10,11,12,13),I
      8  GO TO(4,4,4,5,5,5,6),IG
      9  GO TO(3,3,3,4,4,4,4,5,5,5),IG
      10 GO TO(2,3,3,3,3,4,4,4),IG
      11 GO TO(1,2,2,3,3,3),IG
      12 IF ((I4+IG+I7-3)15,15,16
      13 IF ((I4-2)14,14,1
      14 IL=I+I7
      GO TO(15,1),IL
      15 P=0.0
      RETURN
      16 GO TO(1,2),IG
      1  P=0.0
      22 IF ((I4-2)20,21,20
      2  P=1.0
      2  GO TO 22
      3  P=2.0
      3  GO TO 22
      4  P=3.0
      4  GO TO 22
      5  P=4.0
      5  GO TO 22
      6  P=5.0
      6  GO TO 22
      21 P=P+1.0
      20 RETURN
      END

```

```
* FORTRAN          FUNCTION Q2 CALLED Q2.
*
C
FUNCTION Q2(I1,I2,I3,I4,I5,I6,I7,
IF(I4-2)200,100,200
100 Q2=17
      RETURN
200 I=I1+I2
      GO TO (1,2,3,4,5,6),I
1   GO TO (6,8,7,7,8,6,7,7),I3
2   GO TO (7,8,6,6,8,7,8,6,7,7,8,6),I3
3   GO TO (7,7,8,6,7,6,8,7),I3
4   GO TO (6,7,7,7,8,6),I3
5   GO TO (6,7),I3
6   Q2=0.
      RETURN
7   Q2=1.
      RETURN
8   Q2=2.
      RETURN
END
```

```

*      FORTRAN  S2(I1,I2,I3,I4,I5,I6,I7)
  IF(I4-2)1,100,1
  1  I=I1+I2
      GO TO (2,3,4,5,6,7),I
  2  GO TO (8,9,9,10,7,7,10,9),I3
  3  GO TO (10,7,7,8,9,9,8,9,10,7,7),I3
  4  GO TO (9,10,7,7,10,8,9,9),I3
  5  GO TO (7,9,9,10,7,7),I3
  6  GO TO (7,9),I3
  7  S2=0.0
      RETURN
  8  S2=1.5
      RETURN
  9  S2=.5
      RETURN
 10  S2=1.
      RETURN
 100 I=I1+I2
      GO TO (101,102,103,104,105,112),I
 101 IF(I3-1)107,108,107
 106 S2=16
      S2=(S2-1.)/2.
      RETURN
 107 IF(I3-4)7,9,7
 102 IF(I3-1)109,108,109
 109 IF(I3-4)9,110,9
 110 IF(I7-1)7,10,7
 103 IF(I3-2)108,111,108
 111 IF(I7)9,8,9
 104 IF(I3-2)108,110,108
 105 GO TO (112,108),I3
 112 I=I7+1
      GO TO (7,9),I
  END

```

```

*      FORTRAN
      FUNCTION S12(I1,I2,I3,I4,I5,I6,I7)
      IF(I4-2)100,100,200
100  S12=16
      S12=(S12-1.)/2.
      RETURN
200  I=I1+I2
      GO TO (1,2,3,4,5,6),I
1     GO TO (7,8,8,7,8,8,8,8),I3
2     GO TO (9,6,6,10,9,9,6,9,6,6),I3
3     GO TO (8,7,8,8,7,8,8),I3
4     GO TO (6,9,6,9,6,6),I3
5     GO TO (8,8),I3
6     S12=0.
      RETURN
7     S12=1.5
      RETURN
8     S12=.5
      RETURN
9     S12=1.
      RETURN
10    S12=2.
      RETURN
END

```

```

*          FUNCTION FPC(A,B,C,D,E)
*          N=A+1.0
*          GO TO(1,2,4,5,6,7),N
1   FPC=0.0
    GO TO50
2   FPC=1.0
    GO TO50
3   FPC=0.0
    M=B+1.0
    GO TO(8,9),M
8   IF(C)10,11,10
11  L=E+1.0
    GO TO(12,13,14),L
12  FPC=0.0
    GO TO50
13  FPC=2.0/9.0
    GO TO50
14  FPC=0.0
    GO TO50
15  FPC=0.0
    GO TO50
10  L=E+1.0
    GO TO(15,16,17),L
15  FPC=0.0
    GO TO50
16  FPC=5.0/18.0
    GO TO50
9   L=E+1.0
    GO TO(18,19,19),L
18  FPC=1.0
    GO TO50
19  FPC=0.5
    GO TO50
5   L=C+1.0
    GO TO(20,21,22),L
20  M=E+1.0

```

00	0000	01	0001
1	0001	02	0002
2	0002	03	0003
3	0003	04	0004
4	0004	05	0005
5	0005	06	0006
6	0006	07	0007
7	0007	08	0008
8	0008	09	0009
9	0009	10	0010
10	0010	11	0011
11	0011	12	0012
12	0012	13	0013
13	0013	14	0014
14	0014	15	0015
15	0015	16	0016
16	0016	17	0017
17	0017	18	0018
18	0018	19	0019
19	0019	20	0020
20	0020	21	0021
21	0021	22	0022
22	0022	23	0023
23	0023	24	0024
24	0024	25	0025
25	0025	26	0026
26	0026	27	0027
27	0027	28	0028
28	0028	29	0029
29	0029	30	0030
30	0030	31	0031
31	0031	32	0032
32	0032	33	0033
33	0033	34	0034

```

GO T0(23,24,23),N.
23 FPC=0.0
24 GO T050
24 FPC=1.0/3.0
24 GO T0 50
21 M=E+1.0
21 GO T0(25,26,26),M
25 FPC=1.0
25 GO T050
26 FPC=0.25
26 GO T050
22 M=E+1.0
22 GO T0(27,28,29),M
27 FPC=0.0
27 GO T050
28 FPC=5.0/12.0
28 GO T050
29 FPC=0.75
29 GO T050
6 L=C+1.0
6 GO T0(30,31,32),L
30 FPC=1.0/15.0
30 GO T050
31 FPC=3.0/5.0
31 GO T050
32 FPC=1.0/3.0
32 GO T050
7 FPC=1.0
7 GO T050
50 RETURN
END

```

```

*          FORTRAN          FUNCTION U(A,B,C,D,E,F)
*          P=(2.0*E+1.0)*(2.0*F+1.0)
*          U=SQRTF(P)*W(A,B,C,D,E,F)
*          RETURN
*          END

45          FORTRAN          FUNCTION W(A,B,C,D,E,F)
100          IF(A+B-E)50,101,101
101          IF(A-B+E)50,102,102
102          IF(-A+B+E)50,3,3
3           IF(C+D-E)50,4,4
4           IF(C-D+E)50,5,5
5           IF(-C+D+E)50,6,6
6           IF(A+C-F)50,7,7
7           IF(A-C+F)50,8,8
8           IF(-A+C+F)50,9,9
9           IF(B+D-F)50,10,10
10          IF(B-D+F)50,11,11
11          IF(-B+D+F)50,40,40
40          K=A+B+E+.01
G=K          IF(A+B+E-G)50,41,50
41          K=C+D+E+.01
G=K          IF(C+D+E-G)50,42,50
42          K=A+C+F+.01
G=K          IF(A+C+F-G)50,43,50
43          K=B+D+F+.01
G=K          IF(B+D+F-G)50,44,50
44          P=A-B
Q=C-D
IF(ABSF(P)-ABSF(Q))13,12,12
0152          0065
0153          0066
0154          0067
0155          0068
0156          0069
0070
0071
0072
0073
0074
0075
0076
0077
0078
0079
0080
0081
0082
0083
0084
0085
0086
0087
0088
0089
0090
0091
0092

```

```

12 IF(P)15,14,14
13 IF(Q)17,16,16
14 A1=A
15 B1=B
C1=C
D1=D
GO TO 16
A1=B
B1=A
C1=D
D1=C
GO TO 16
A1=C
B1=D
C1=A
D1=B
GO TO 16
A1=D
B1=C
C1=B
D1=A
GO TO 16
C1=-B1+D1+F
C2=B1-D1+F
C3=B1+D1-F
C4=B1+D1+F+1.
P1=A1-B1
Q1=C1-D1
ALPHA=P1-Q1
BETA=P1+Q1
S=1.0
IF(MODF(CC,2.0)>91,91,90
S=-1.0
XN= 10.**(-30)*SF(E-P1+1.0,E+P1)*SF(CA-ALPHA+1.0,CA)
1 *SF(CB+1.0,CB+ALPHA)*SF(CC+1.0,CC+BETA)*SF(CD+1.0,CD+BETA)
XD=10.0**(-30)*

```

```

1 SF(1.0•E+Q1)*SF( 1.0•E-Q1)*SF(2.0•          *B1-E+P1+1.0•2.0•0*B1+E+P1  0129
2 +1.0)*SF(2.0•D1-E+Q1+1.0•2.0•D1+E+Q1+1.0)  0130
XN=SQRTF(XXN)  0131
XD=SQRTF(XXD)  0132
N=S*XN/XD  0133
WA=0.0  0134
Z=0.0  0135
SZ=1.0  0136
92 IF(MODF(Z,2.0)>93,93,94  0137
94 SZ=-1.0  0138
93 DWA=SZ*SF(1.0•E-P1)*SF(Q1+P1+Z+1.0•0•E+Q1)  0139
1*SF(CA-ALPHA-E+P1+Z+1.0•0,CA-ALPHA)  0140
2*SF(CB-E+P1+Z+1.0•CB)*SF(E-Q1-Z+1.0•E-Q1)  0141
3*SF(CC-Z+1.0•CC)*SF(CD+BETA+1.0,CD+BETA+Z) /  0142
4(SF(1.0•E-P1-Z)*SF(1.0,Z))  0143
WA=WA+DWA  0144
Z=Z+1.0  0145
92 IF(E-P1-Z)35,92,92  0146
95 W=W*WA  0147
GO TO 51  0148
50 W=0.0  0149
51 RETURN  0150
END  0151

```

```

* FORTRAN
C   TO ORDER L ELEMENTS IN BUFFER ARRAY B
C   SUBROUTINE BSORT(L)
COMMON J1,J2,J3,J4,J5,J6,J7,J1P,J2P,J3P,J4P,J5P,J6P,J7P,IBETA,
1  INCASE,ALPHAO,ALPHA,E, ID1, ID2, B,NREC, LTOT, NTOT,NDIM
DIMENSION ALPHA(1500,6),E(1500),ID1(1500),ID2(1500),B(1500,3)
N=L-1
DO 20 I=1,N
NP=I+1
DO 20 J=NP,L
IF(B(I,1)-B(J,1)) 20,20,10
10 DO 15 K=1,3
Y=B(I,K)
B(I,K)=B(J,K)
15 B(J,K)=Y
20 CONTINUE
RETURN
END

```

```

* FORTRAN
* SUBROUTINE ORDER
COMMON J1,J2,J3,J4,J5,J6,J7,J1P,J2P,J3P,J4P,J5P,J6P,J7P,IBETA,
1  NCASE,ALPHAO,ALPHA, E, ID1, ID2, B, NREC, LTOT, NTOT,NDIM
DIMENSION ALPHA(1500,6),E(1500),ID1(1500),ID2(1500),B(1500,3)
WRITE TAPE 25, NCASE, ALPHAO,IBETA, LTOT, NREC, ID1, ID2, E, ALPHA
REWIND 15
REWIND 16
DO 110 I=1,NDIM
ALPHA(I,1)=B(I,1)
ALPHA(I,3)=B(I,2)
ALPHA(I,5)=B(I,3)
110 IF(NREC) 50,50, 100
50 CALL LIST(LTOT)
RETURN
100 NTAPE=1
111 N=NREC
NREC=0
113 GO TO (115, 120),NTAPE
115 READ TAPE 15,B
GO TO 125
120 READ TAPE 16,B
125 DO 150 I=1,NDIM
ALPHA(I,2)=B(I,1)
ALPHA(I,4)=B(I,2)
ALPHA(I,6)=B(I,3)
150 N2DIM=2*NDIM
CALL ASORT(N2DIM)
160 N=N-1
161 IF(N) 250,250,170
170 DO 180 I=1,NDIM
B(I,1)=ALPHA(I,2)
B(I,2)=ALPHA(I,4)
B(I,3)=ALPHA(I,6)
180 NREC=NREC+1
GO TO (190,200),NTAPE

```

190 WRITE TAPE 16,B
GO TO 113
200 WRITE TAPE 15,B
GO TO 113
250 REWIND 15
REWIND 16
CALL LIST(NDIM)
260 LTOT=LTOT-NDIM
DO 270 I=1,NDIM
ALPHA(I,1)=ALPHA(I,2)
ALPHA(I,3)=ALPHA(I,4)
ALPHA(I,5)=ALPHA(I,6)
IF (LTOT-NDIM)50,50,280
280 GO TO (290,295),NTAPE
290 NTAPE=2
GO TO 111
295 NTAPE=1
GO TO 111
END

MPOR 31
MPOR 32
MPOR 33
MPOR 34
MPOR 35
MPOR 36
MPOR 37
MPOR 38
MPOR 39
MPOR 40
MPOR 41
MPOR 42
MPOR 43
MPOR 44
MPOR 45
MPOR 46
MPOR 47
MPOR 48
MPOR E

```

* FORTRAN
SUBROUTINE LIST(N)
COMMON J1,J2,J3,J4,J5,J6,J7,J1P,J2P,J3P,J4P,J5P,J6P,J7P,IBETA,
1 NCASE,ALPHAO,ALPHA,E, ID1, ID2, B,NREC, LTOT, NTOT,NDIM
1 DIMENSION ALPHA(1500,6),E(1500),ID1(1500),ID2(1500),B(1500,3)
1 WRITE TAPE 25,(ALPHA(J,1),ALPHA(J,3),ALPHA(J,5),J=1,N)
1 RETURN
1 END

```

```

MPLI 0
MPLI C1
MPLI C2
MPLI D1
MPLI 1
MPLI 14
MPLI E

```

```

* FORTRAN
SUBROUTINE ASORT(L)
COMMON J1,J2,J3,J4,J5,J6,J7,J1P,J2P,J3P,J4P,J5P,J6P,J7P,JBETA,
1 NCASE,ALPHAO,ALPHA, E, ID1, ID2, B,NREC, LTOT, NTOT,NDIM
DIMENSION ALPHA(1500,6),E(1500),ID1(1500),ID2(1500),B(1500,3)
N=L-1
DO 30 I=1,N
NP=I+1
DO 20 J=NP,L
IF (ALPHA(I,1)-ALPHA(J,1)) 20,20,10
10 Y=ALPHA(I,1)
ALPHA(I,1)=ALPHA(J,1)
ALPHA(J,1)=Y
Y=ALPHA(I,3)
ALPHA(I,3)=ALPHA(J,3)
ALPHA(J,3)=Y
Y=ALPHA(I,5)
ALPHA(I,5)=ALPHA(J,5)
ALPHA(J,5)=Y
20 CONTINUE
30 CONTINUE
RETURN
END
* MPAS 0
NP C1
NP C2
NP D1
NPAS 1
NPAS 2
NPAS 3
NPAS 4
NPAS 5
NPAS 6
NPAS 7
NPAS 8
NPAS 9
NPAS 10
NPAS 11
NPAS 12
NPAS 13
NPAS 14
NPAS 15
NPAS 16
NPAS 17
NPAS F

```

```

* FORTRAN
  SUBROUTINE TWRITE
  SUBROUTINE TWRITE TO PREPARE FINAL TRANSITION TAPE - 13 WORDS PER
  C
  1RECORD
  COMMON J1,J2,J3,J4,J5,J6,J7,J1P,J2P,J3P,J4P,J5P,J6P,J7P,IBETA,N
  1CASE,ALPHAO,ALPHA,E,IDL,IDL2,B,NREC,LTOT,NTOT,NDIM
  DIMENSION ALPHA(1500,6),E(1500),IDL(1500),IDL2(1500),B(1500,3)
  REWIND 25
  REWIND 16
  NR=1
  2 READ TAPE 25,NCASE,ALPHAO,IBETA,LTOT,NREC,IDL,IDL2,E,ALPHA
  WRITE TAPE 16,NCASE,ALPHAO,IBETA,LTOT,NDIM
  LINE=50
  5 IF(LTOT-NDIM)15,15,10
  10 N=NDIM
  GO TO 20
  15 N=LTOT
  20 READ TAPE 25,(B(L,1),B(L,2),B(L,3),L=1,N)
  DO 30 L=1,N
  K=B(L,3)/2000.0
  I=B(L,3)-2000.0*FLOATF(K)
  WRITE TAPE 16,B(L,1),B(L,2),ID1(I),ID2(I),E(I),IDL(K),IDL2(K),ALPH
  1A(I,J),J=1,6)
  30 CONTINUE
  LTOT=LTOT-NDIM
  IF(LTOT)56,56,5
  56 NR=NR+1
  IF(NR-NTOT) 2, 2,60
  60 REWIND 25
  END FILE 16
  REWIND 16
  RETURN
  END

```

```

* FORTRAN
* SUBROUTINE MSET
C SET UP TABLES FOR MULTIPET II-
COMMON ABSMIN, TEMP, NENGY, DENS, NSLIM, NMAX, WFACT, LTOT, K1,K2,MULT
1 1GI, NI, LI, KSI, LAI, NSI, NPI, L12I, IS12I, IGF, NF, LF, KSF, MULT
2 LAF, NSF, NPF, L12F, IS12F, DELTAE, Z, ALPHA, FNO, SIGSQ, GFACT, MULT
3 WCOLL, WDOPP, EI, XMCSQ, DENMIN, NMAX,
4 ASLATE, BSLATE, CSLATE, A,B, FSHELL, SERLIM
DIMENSION DENS(2,6), NSLIM(6), ALPHA(6),
1 ASLATE(28,36,2), BSLATE(28,7,36), CSLATE(24,36), A(8,8,16),
2 B(8,8,16), FSHELL(8,8), SERLIM(11,12,2)
10 READ INPUT TAPE 5, 1000, ABSMIN, TEMP, NENGY
20 READ INPUT TAPE 5, 1020, ((DENS(I,J),J=1:6),I=1,2)
30 DO 35 J=1,6
35 DENS(1,J)=1.74676E-17*DENS(1,J)*6.28318
DENMIN=MIN1F(DENS(2,1),DENS(2,2),DENS(2,3),DENS(2,4),DENS(2,5),
1 DENS(2,6))
40 DO 45 J=1,6
X=(4.107E22*SQRTF(TEMP)/DENS(2,J))**(1./7.)
IF(X-7.0)41,41,42
41 NSLIM(J)=7
GO TO 45
42 NSLIM(J)=X+0.50
45 CONTINUE
50 NMAX=XMAXOF(NSLIM(1),NSLIM(2),NSLIM(3),NSLIM(4),NSLIM(5),NSLIM(6))
CALL TREAD
WFACT=.637E-23/SQRTF(TEMP)
RETURN
1000 FORMAT(2E20.8,110)
1020 FORMAT(6E12.6)
END

```

```

* FORTRAN
SUBROUTINE TREAD
COMMON ABSMIN, TEMP, NENGY, DENS, NSLIM, NMAX, WFACT, LTOT, K1,K2,MULT
 1 10
 1 IGI, NI, LI, KSI, LAI, NSI, NPI, L121, IS121, IGF, NF, LF, KSF, MULT
 2 LAF, NSF, NPF, L12F, IS12F, DELTAE, Z, ALPHA, FNO, SIGSQ, GFACT,MULT
 3 WCOLL, WDOPP, EI, XMCSQ, DENMIN, NMAX,
 4 ASLATE, BSLATE, CSLATE, A,B, FSHELL, SERLIM
 5 MULT 1C1
 5 DIMENSION DENS(2,6), NSLIM(6), ALPHA(6),
 1 ASLATE(28,36,2), BSLATE(28,7,36), CSLATE(24,36), A(8,8,16),
 2 EI(8,8,16), FSHELL(8,8), SERLIM(11,12,2)
 80 MULT 2D1
REWIND 26
 90 READ TAPE 26,ASLATE,BSLATE,CSLATE
CALL SFIL(26,1)
 100 READ TAPE 26,A,B
 110 CALL SFIL(26,1)
 120 READ TAPE 26,FSHELL,SERLIM
 130 RETURN
 140 END
 150

```

```

*   FORTRAN
*   SUBROUTINE ATLAS-  EVALUATE F-NUMBERS AND LINE WIDTHS-
C   COMPILE LINE ATLAS-  COMMON ABSMIN, TEMP, NENGY, DENS, NSLIM, NMAX, WFACT, LTOT, K1,K2,00000030
COMMON ABSMIN, TEMP, NENGY, DENS, NSLIM, NMAX, WFACT, LTOT, K1,K2,00000030
1  IGI, NI, LI, KSI, LAI, NSI, NPI, L12I, IS12I, IGF, NF, LF, KSF, 00000040
2  LAF, NSF, NPF, L12F, IS12F, DELTAE, Z, ALPHA, FNO, SIGSQ, GFACT, 00000050
3  WCOLL, WDOPP, EI, XMCSG, DENMIN, NMAX, 00000060
4  ASLATE, BSLATE, CSLATE, A,B, FSHELL, SERLIM, 00000070
DIMENSION DENS(2,6), NSLIM(6), ALPHA(6), 00000080
1  ASLATE(28,36,2), BSLATE(28,7,36), CSLATE(24,36), A(8,8,16),
2  B(8,8,16), FSHELL(8,8), SERLIM(11,12,2),FPW(6) 00000090
REWIND 15 00000100
REWIND 16 00000110
10  READ TAPE 16,NCASE, ALPHA, IBETA, LTOT, NDIM 00000120
WRITE TAPE 15, LTOT, NCASE, ALPHA0, IBETA 00000130
LINE=50 00000140
DO 300 L=1,LTOT 00000150
20  READ TAPE 16, DELTAE, Z, ID1I, ID2I, EI, ID1F, ID2F, ALPHA 00000160
30  K1=ID1I/1000 00000170
      K2=(ID1I-1000*K1)/100 00000180
      IGI=ID1I-1000*K1-100*K2 00000190
      NI=ID2I/1000 00000200
      LI=(ID2I-1000*NI)/100 00000210
      KSI=(ID2I-1000*NI-100*LI)/100 00000220
      LAI=ID2I-1000*NI-100*LI-10*KSI 00000230
      NSI=0(K1,K2,IGI,NI,LI,KSI,LAI) 00000240
      NPI=P(K1,K2,IGI,NI,LI,KSI,LAI) 00000250
      L12I=Q2(K1,K2,IGI,NI,LI,KSI,LAI) 00000260
      IS12I=S12(K1,K2,IGI,NI,LI,KSI,LAI)*2.0+1.0 00000270
      IGF=ID1F-1000*K1-100*K2 00000280
      NF=ID2F/1000 00000290
      LF=(ID2F-1000*NF)/100 00000300
      KSF=(ID2F-1000*NF-100*LF)/10 00000310
      LAF=ID2F-1000*NF-100*LF-10*KSF 00000320
      NSF=0(K1,K2,IGF,NF,LF,KSF,LAF) 00000330
      NPF=P(K1,K2,IGF,NF,LF,KSF,LAF) 00000340
      0N700350

```

```

L12F=Q2(K1,K2,IGF,NF,LF,KSF,LAF)
1512F=S12(K1,K2,IGF,NF,LF,KSF,LAF)*2.0+1.0
47 FNO=0.0
SIGSQ=0.0
IF(DELTAE)250,250,100
100 CALL FCALC
150 IF(FNO) 160, 160, 200
160 IF(LINE-50)163,161,161
161 WRITE OUTPUT TAPE 6,162
162 FORMAT(1H1)
LINE=0
163 WRITE OUTPUT TAPE 6, 1000, DELTAE, Z, ID1I, ID2I, EI, ID1F, IF-
1 FNO, SIGSQ, GFACT, WCOLL, WDOPP
LINE = LINE+3
GO TO 250
200 CALL WIDTH
IF(WCOLL) 160, 160, 250
250 WRITE TAPE 15, DELTAE, Z, FNO, SIGSQ, GFACT, WCOLL, WDOPP, ID1I,
1 ID2I, EI, ID1F, ID2F, ALPHA, XMC5Q
DO 299 J=1,6
FW(J)=FNO*ALPHA(J)*DENS(1,J)/(DENS(2,J)*3.141592653*WCOLL)
299 CONTINUE
EIF=DELTAE-#1
IF(LINE-50)1203,1201,1201
1201 WRITE OUTPUT TAPE 6,1202
1202 FORMAT(1H1,2X,7HDELTA E,12X,3HFNO,11X,7HSIGMASQ,9X,7HW(COLL),9X,7H00000610
1W,DOPP),6X,6HID (1),8X,2HEI,9X,6HID (F),8X,2HEF/1H,12X,6HF1/PIW,100000620
20X,6HF2/PIW,10X,6HF3/PIW,10X,6HF4/PIW,13X,6HF5/PIW,13X,6HF6/PIW/1H00000630
30)
LINE=4
1203 WRITE OUTPUT TAPE 6,1204,DELTAE,FNO,SIGSQ,WCOLL,WDOPP, ID1I, ID2I, EI, ID1F, ID2F, EF, (FW(J),J=1,6)
1204 FORMAT(1H0,1PE14.7,4E16.7,215, 1PE15.7,215, 1PE14.7/E24.7,3E16.7,200000680
1E19.7)
LINE=LINE+3
300 CONTINUE

```

```
320 END FILE 15
325 REWIND 15
326 REWIND 16
327 RETURN
1000 FORMAT(17H FNO/WCOLL ERROR-/1P2E12.4,I10,I5,E12.4,I10,I5/5E12.4)
END
```

```
00000720
00000730
00000740
00000750
00000760
00000770
```

```

      FORTRAN
      SUBROUTINE FCALC
      C EVALUATES F-NUMBER FOR SPECIFIED TRANSITION-
      COMMON ABSMIN, TEMP, NENGY, DENS, NSLIM, NMAX, WFACT, LTOT, K1,K2,00000032
      1 1GI, NI, LI, KSI, LAI, NSI, NPI, L12I, IS12I, IGF, NF, LF, KSF, 00000042
      2 LAF, NSF, NPF, L12F, IS12F, DELTAE, Z, ALPHA, FNO, SIGSQ, GFACT, 00000052
      3 WCOLL, WDOPP, EI, XMCSQ, DENMIN, NMAX, 00000062
      4 ASLATE, BSLATE, CSLATE, A,B, FSHELL, SERLIM, 00000072
      DIMENSION DENS(2,6), NSLIM(6), ALPHA(6), 00000082
      1 ASLATE(28,36,2), BSLATE(28,7,36), CSLATE(24,36), A(8,8,16), 00000092
      2 B(8,8,16), FSHELL(8,8), SERLIM(11,12,2), 00000102
      IF((IGI-IGF) 50, 10, 50 00000112
      10 DO 20 J=1,6 00000122
      11 IF(INF-NSLIM(J)) 20, 15, 15 00000132
      15 ALPHA(J)=0.0 00000142
      20 CONTINUE 00000152
      50 IF(NI=16) 60, 60, 80 00000162
      60 NZERO=XMINOF(NI,9) 00000172
      GO TO ( 80, 150, 200, 250, 250, 250, 400),NZERO 00000182
      80 FNO=0.0 00000192
      I=0 00000202
      100 IF(I) 125, 125, 110 00000212
      110 GO TO ( 112, 114, 116, 118, 120),I 00000222
      112 GFACT=(2*LAI+1)*KSI 00000232
      GO TO 122 00000242
      114 GFACT=KSI*(2*L12I+1)*(2*LI+1) 00000252
      GO TO 122 00000262
      116 GFACT=2*(2*LI+1)*IS12I *(2*L12I+1) 00000272
      GO TO 122 00000282
      118 GFACT=2*(NI*NI-16)*IS12I *(2*L12I+1) 00000292
      GO TO 122 00000302
      120 GFACT=2*NI*NI*IS12I *(2*L12I+1) 00000312
      122 FNO=DELTAE/13.605*Z/GFACT*SIGSQ/3.0 00000322
      125 RETURN 00000332
      150 IF(INF-9) 160, 80, 80 00000342
      160 I=1 00000352

```

```

170 SIGSQ=SLATER(K1,K2, NSI, NPI, NI,LI, NSF, NPF, NF, LF)
175 IF(SIGSQ) 175, 175, 100
175 I=0
FNO=FHYDRO(NI, LI, NF, LF)
GO TO 100
200 IF(NF-9) 210, 80, 80
210 IF(LAI-9) 160, 220, 160
220 I=2
GO TO 170
250 IF(NF-16) 260, 260, 80
260 IF(IGI-IGF) 270, 300, 270
270 IF(LI-4) 275, 280, 280
275 I=3
GO TO 170
280 I=4
SIGSQ=SLATER(K1,K2, NSI,NPI, NI, 3, NSF,NPF, NF, 3)
IF(SIGSQ) 290, 290, 100
290 I=0
FNO=FHYDRO(NI, 3, NF, 3)
GO TO 100
300 IF(NF-9) 310, 350, 350
310 IF(LI-4) 320, 330, 330
320 IF(LF-LI+1) 322, 275, 322
322 IF(LI-3) 275, 325, 325
325 I=0
FNO=FHYDRO(NI, LI, NF, LI+1)
GO TO 100
330 I=0
X=NI*NI-16
M=NI-1
DO 335 LZERO=4,M
Y=2*LZERO+1
335 FNO=FNO+Y*(FHYDRO(INI,LZERO,NF,LZERO-1),
1 +FHYDRO(INI,LZERO,NF,LZERO+1))
FNO=FNO/K
GO TO 100
00000362
00000372
00000382
00000392
00000402
00000412
00000422
00000432
00000442
00000452
00000462
00000472
00000482
00000492
00000502
00000512
00000522
00000532
00000542
00000552
00000562
00000572
00000582
00000592
00000602
00000612
00000622
00000632
00000642
00000652
00000662
00000672
00000682
00000692
00000702
00000712

```

350 IF(LI=4) 360, 330, 330
360 I=0
FNO=FHYDRO(NI,LI,NF,LI-1)+FHYDRO(NI,LI,NF,LI+1)
GO TO 100
400 IF(IGI-IGF) 420, 410, 420
410 I=0
FNO=FSHELL(NF-8, NI-8)
GO TO 100
420 I=5
SIGSQ=SLATER(K1,K2, NS!,NPI,8, 3, NSF, NPF, 8, 3)
IF(SIGSQ) 425, 425, 100
425 I=0
FNO=FHYDRO(2,0,2,1)
GO TO 100
END
00000722
00000732
00000742
00000752
00000762
00000772
00000782
00000792
00000802
00000812
00000822
00000832
00000842
00000852
00000862

```

* * * * *
      FORTran
      LIST
      *
      * FUNCTION SLATER(IXM1,IXM2,IYM,NM,LM,IYPM,IYPM,NPM,LPM)
      COMMON ABSMIN, TEMP, NENGY, DENS, NSLIM, NMAX, WFACT, LTOI, K1,K2,00000030
      1  IGI, NI, LI, KSI, LAI, NSI, NPI, L121, IS121, IGF, NF, LF, KSF, 00000040
      2  LAF, NSF, NPF, L12F, IS12F, DELTAE, Z, ALPHA, FNO, SIGSQ, GFACT, 00000050
      3  WCOLL, WDOPP, EI, XMCSQ, DENMIN, NMAX, 00000060
      4  ASLATE, BSLATE, CSLATE, A,B, FSHELL, SERLIM, 00000070
      DIMENSION DENS(2,6), NSLIM(6), ALPHA(6), 00000080
      1  ASLATE(28,36,2), BSLATE(28,7,36), CSLATE(24,36), A(8,8,16), 00000090
      2  B(8,8,16), FSHELL(8,8), SERLIM(11,12,2), 00000100
      IX1=IXM1, 00000110
      IX2=IXM2, 00000120
      IY=IYM, 00000130
      NM=NM, 00000140
      LM=LM, 00000150
      IXP=IYPM, 00000160
      IYP=IYPM, 00000170
      NP=NPM, 00000180
      LP=LP, 00000190
      IF((N-NP)3,1,3, 00000200
      1  IF((LP-L)2,3,3, 00000210
      2  IXT1=IXP, 00000220
      IYT1=IYP, 00000230
      NT1=NP, 00000240
      LT1=LP, 00000250
      IXP=IX, 00000260
      IYP=IY, 00000270
      NP=N, 00000280
      LP=LP, 00000290
      IX=IXT1, 00000300
      IY=IYT1, 00000310
      NZ=NT1, 00000320
      L=LT1, 00000330
      3  IF((N-2)2000,5000,2000

```

```

5000 IF (L-1) 1500,1000,1500
1000 N=0
L=0
12=0
GO TO 2000
1500 I2=0
L=0
N=0
2000 IF (NP-2) 4000,2500,4000
2500 IF (LP-1) 3500,3000,3500
3000 NP=0
LP=0
IZP=0
GO TO 4000
3500 IZP=0
LP=0
NP=0
4000 IF (N-8) 503,503,45
503 IF (NP-8) 504,504,45
504 J=6*I*14*I*2
IF (N-NP) 15,11,15
11 IF (L-LP) 15,12,15
12 IF (N) 130,13,130
13 IF (L) 130,15,130
C OPTION A
15 IF (IX-IXP) 180,20,80
20 IX=IX
IF (IY-IYP) 35,25,35
25 IETA=IY
NEP=N
LB=LB
NEIP=NP
LEIP=LP
27 IC1=12*I*1+J
IF (NB-NBF) 165,30,65
30 IS=(3+LB)*LB/2

```

```

K1S=7*LB+(NB-1)
SLATER=ASLATE(K1S,IC1,IS)
GO TO 140
35 IF(I2)45,40,55
40 IETA=IY-1
NB=2
LB=1
NBP=NP
LBP=LP
IF(IY-IETA)45,27,45
45 WRITE OUTPUT TAPE 6,50,I2B,IX,IY,N,L,IZ,IXP,IYP,NP,LP,I2P
50 FORMAT(1H0,2X,17HERROR IN INPUT - 11,10H 102 2011,4H 2111,2X,300000830
111,5X,7H102 2011,4H 2111,2X,311)
GO TO 140
55 IF(I2P)45,60,45
60 IETA=IY-1
NBP=2
LBP=1
NB=N
LB=L
IF(IY-IETA)45,27,45
65 IF(LBP-(LB-1))70,75,70
70 N1B=NBP
L1B=LBP
NBP=NBP
LBP=L
NB=N1B
LB=L1B
75 K2S=7*LB+(NB-1)
NBP1=NBP-1
SLATER=BSLATE(K2S,NBPM1,IC1)
GO TO 140
80 IF(IY-IYP)105,85,105
85 IETA=IY
IF(I2)45 90,95
90 NB=2
00000720
00000730
00000740
00000750
00000760
00000770
00000780
00000790
00000800
00000810
00000820
00000830
00000840
00000850
00000860
00000870
00000880
00000890
00000900
00000910
00000920
00000930
00000940
00000950
00000960
00000970
00000980
00000990
00001000
00001010
00001020
00001030
00001040
00001050
00001060
00001070

```

```

LB=0
IXI=IX-1
NBP=NP
LBP=LP
92 IF(IXI-IXP)45,27,45
95 IF(I2P)45,100,45
100 IXI=IXP-1
NBP=2
LBP=0
NB=N
LB=L
102 IF(I2I-IX)45,27,45
105 IF(I2)45,110,130
110 IF(I2P)45,15,130
115 IF(IX-IXP)120,20,125
120 IXI=IXP-1
NBP=2
LBP=0
IETA=IY-1
NB=2
LB=1
125 IXI=IX-1
NB=2
LB=0
IETA=IY-1
NBP=2
LBP=1
IF(IETA-IY)45,102,45
OPTION B
130 IF(N-3)45,135,135
135 IC2=12*I X +
K=6*L+(N-2)
SLATER=CSLATE(K,IC2)
140 RETURN
END

```

```

*      FORTRAN FHYDRO(N,L,LP)
      FUNCTION FHYDRO(N,L,LP)
      COMMON ABSMIN, TEMP, NENY, DENS, NSLIM, NMAX, WFACT, LTOT, K1,K2,MULT
      10      30      1CT
      1  IGI, N1, LI, KSI, LAI, NSI, NPI, L12I, IS12I, 1GF, NF, LF, KSF, MULT 2CT
      2  LAF, NSF, NPF, L12F, IS12F, DELTAE, Z, ALPHA, FNO, SIGSQ, GFACT, MULT 3CT
      3  WCOLL, WDOPP, EI, XMCSSQ, DENMIN, NMAX, MULT 4CT
      4  ASLATE, BSLATE, CSLATE, A,B, FSHELL, SERLIM MULT 1C1
      DIMENSION DENS(2,6), NSLIM(6), ALPHA(6), MULT 1D1
      1  ASLATE(28,36,2), BSLATE(28,7,36), CSLATE(24,36), A(8,8,16),
      2  B(8,8,16), FSHELL(8,8), SERLIM(11,12,2) MULT 2D1
      60
      L2I=L+1
      70
      IF(L-LP)6,7,5
      80
      90
      100
      110
      120
      130
      140
      150
      5  FHYDRO=A(N,LP1,NP)
      GO TO 15
      6  FHYDRO=B(N,LP1,NP)
      GO TO 15
      7  WRITE OUTPUT TAPE 6,10,N,L,LP,NP,LP
      10  FORMAT(1H0,2X,13HERROR L=LP,N=11,2X,2HL=11,2X,3HNP=11,2X,3HLP=11)
      15  RETURN
      END

```

```

*   FORTRAN
*   SUBROUTINE WIDTH
C   EVALUATE COLLISION AND DOPPLER HALF-WIDTHS OF TRANSITION-
COMMON ABSMIN, TEMP, NENGY, DENS, NSLIM, NMAX, WFACT, LTOT, K1,K2,MULT 1CT
1  IGI, NI, LI, KSI, LAI, NSI, NPI, L12I, IS12I, IGF, NF, LF, KSF, MULT 2CT
2  LAF, NSF, NPF, L12F, IS12F, DELTAE, Z, ALPHA, FNO, SIGSQ, GFACT, MULT 3CT
3  WCOLL, WDOPP, EI, XMCSQ, DENMIN, NMAX, WIDTH 0
4  ASLATE, BSLATE, CSLATE, A,B, FSHELL, SERLIM, WIDTH C1
DIMENSION DENS(2,6), NSLIM(6), ALPHA(6), WIDTH C1
1  ASLATE(28,36,2), BSLATE(28,7,36), CSLATE(24,36), A(8,8,16), MULT 1DT
2  R(8,8,16), FSHELL(8,8), SERLIM(11,12,2), MULT 2D1
XMCSQ=18.62E+8*FLOAT(8-K1) WIDTH 10
WDOPP= DELTAE*SQRTF(2.0*TEMP/XMCSQ) WIDTH 20
J=6*K1+K2 WIDTH 30
ZRES=K2*K2 WIDTH 40
IF (NI-NF)150,10*50 WIDTH 50
10  IF (LI-LF)150,20*50 WIDTH 60
20  XNUSQ=SERLIM(J,IGF,2)**2/ZRES WIDTH 70
IF (XNUSQ-1.0) 22, 22, 24 WIDTH 80
22  Y=0.0 WIDTH 90
GO TO 100 WIDTH 100
24  Y=3.0 WIDTH 110
GO TO 100 WIDTH 120
50  XNUSQ=13.605/(SERLIM(J,IGF,1)-DELTAE-EI) WIDTH 130
IF (NF-9) 70, 60, 60 WIDTH 140
60  Y=NF*NF-1 WIDTH 150
GO TO 100 WIDTH 160
70  IF (LF-4) 80, 90, 90 WIDTH 170
80  Y=3*LF*(LF+1) WIDTH 180
GO TO 100 WIDTH 190
90  Y=NF*NF-1+4*(NF+4) WIDTH 200
100 WCOLL=WFACT*XNUSQ*(5.0*XNUSQ*ZRES+1.0-Y) WIDTH 210
RETURN
END

```

```

*   FORTRAN ABS
C   EVALUATE ABSORPTION COEFFICIENT DUE TO BROAD LINES IN LINE ATLAS-
C   NARROW LINES ACCUMULATED IN PLANCK MEAN-
COMMON ABSMIN, TEMP, NENGY, DENS, NSLIM, NMAX, WFACT, LTOT, K1, K2, MULT 1CT
1  IGI, NI, LI, KSI, LAI, NSI, NPI, L121, IS121, IGF, NF, LF, KSF, MULT 2CT
2  LAF, NSF, NPF, L12F, IS12F, DELTAE, Z, ALPHA, FNO, SIGSQ, GFACT, MULT 3CT
3  WCOLL, WDOPP, EI, XMCSQ, DENMIN, NMAX, MULT 4CT
4  NOMEA, OMEGA0, DOMEA, OMEGA, ABS, PSI1, PSI2, PSI
DIMENSION DENS(2,6), NSLIM(6), ALPHA(6),
1  OMEGA(2000), ABS(2000,6), AB(6), PSI1(17), PSI2(8), PSI1(17,8)
REWIND 15
REWIND 25
READ INPUT TAPE 5,1500,PSI2, PSI1, PSI
10 DO 600 NEN=1,NENGY
20 READ INPUT TAPE 5, 1000, NOMEA, OMEGA0, DOMEGA
DO 30 J=1,6
30 AB(J)=0.0
DO 40 N=1,NOMEA
OMEGA(N)=OMEGA0+FLOATF(N-1)*DOMEGA
DO 35 J=1,6
35 ABS(N,J)=0.0
40 CONTINUE
50 READ TAPE 15, LTOT, NCASE, ALPHA0, IBETA
NCENT=2
100 DO 500 LCOUNT=1,LTOT
READ TAPE 15, DELTAE, Z, FNO, SIGSQ, GFACT, WCOLL, WDOPP, ID11,
1  ID21, EI, ID1F, ID2F, ALPHA, XMCSQ
120 IF(OMEGA0-DELTAE) 140, 130, 130
130 OMEGAC=DELTAE
N=1
IFLAG=1
GO TO 200
140 DO 150 NCENT, NOMEA
IF(OMEGA(N)-DELTAE) 150, 160, 160
150 CONTINUE

```

```

OMEGAC=DELTAE
N=OMEGAC
NCENT=N
IFLAG=0
GO TO 200
160 IF(OMEGA(N)-DELTAE-ABSF(DELTAE-OMEGA(N-1))) 170, 170, 180
170 OMEGAC=OMEGA(N)
NCENT=N
GO TO 190
180 OMEGAC=OMEGA(N-1)
NCENT=N-1
N=N-1
190 IFLAG=0
200 DO 400 J=1,6
210 IF(ALPHA(J)) 400, 400, 210
210 ALPHA(J)=ALPHA(J)*DENS(1,J)
Y=NCOLL*DENS(2,J)*10.0
220 IF(2.0*Y-OMEGA) 230, 240, 240
230 IF(OMEGA0-DELTAE) 232, 232, 400
232 IF(OMEGA(N-1)-DELTAE) 400, 235, 235
235 AB(J)=AB(J)+LPHA(J)*FNO*DELTAE**3*EXPF(-DELTAE/TEMP)
GO TO 400
240 NQ=N
1Q=IFLAG
ETA=WDOPP/Y
250 X=(OMEGA(NQ)-OMEGAC)/Y
1F(ETA-0.2) 280, 280, 260
260 IF(ABSF(X)/ETA-5.0) 270, 280, 280
270 B=1.0/(3.14159*Y)*VOIGT(X,ETA, )
GO TO 300
280 B=1.0/(6.28318*Y)*(1.0/(1.0+(X+0.7071*ETA)**2)+1.0/(1.0+(X-
1
1*7071*ETA)**2))
300 XABS=ALPHA(J)*FNO*B
IF(XABS-ABSMIN*ABS(NQ,J)) 310, 330, 330
310 IF(IQ) 320, 320, 400
320 NQ=NCENT

```

```

1000  IQ=1
1000  GO TO 340
1000  ABS(NQ,J)=AB5(NQ,J)+XABS
1000  IF(IQ) 350, 350, 340
1000  NQ=NQ+1
1000  IF(NQ-NOMEGA) 250, 250, 400
1000  NQ=NQ-1
1000  IF(NQ) 320, 320, 250
1000  CONTINUE
1000  CONTINUE
1000  REWIND 15
1000  DO 510 J=1,6
1000  AB(J)=15399/TEMP**4*AB(J)
1000  WRITE OUTPUT TAPE 6, 1200, OMEGA0,OMEGA,OMEGA(NOMEGA),AB
1000  CALL TALLY
1000  CONTINUE
1000  RETURN
1000  FORMAT(110, 2E20.8)
1100  FORMAT(42H1 NARROW LINE CONTRIBUTION TO PLANCK MEAN-,20X,7HENERGY=ABS
1100  1,1PE9.3,1H1,1PE9.3,1H1,1PE9.3/6E20.6)
11500 FCRMAT(8F5.4/17F4.1/(17F4.4))

```

```

*   FORTRAN
*   FUNCTION VOIGT(X,ETA, )
C   EVALUATE VOIGT LINE PROFILE-
COMMON ABSMIN, TEMP, NENGY, DENS, NSLIM, NMAX, WFACT, LTOT, K1,K2,MULT 1CT
1  IGI, NI, LI, KSI, LAI, NSI, NPI, L121, IS121, IGF, NF, LF, KSF, MULT 2CT
2  LAF, NSF, NPF, L12F, IS12F, DELTAE, Z, ALPHA, FNO, SIGSQ, GFACT, MULT 3CT
3  WCOLL, WDOPP, EI, XMCSQ, DENMIN, NMAX, MULT 4CT
4  NOMEA, OMEGA, DOMEA, OMEGA, ABS, AB, PSI1, PSI2, PSI
DIMENSION DENS(2*6), NSLIM(6), ALPHA(6),
1  OMEGA(2000), ABS(2000,6), AB(6), PSI1(17), PSI2(8), PSI(17,8)
60  ETA=MIN1(ETA,5.0)
DO 75 N=2,8
    IF(ETA-PSI2(N)) 100, 100, 75
75  CONTINUE
N=8
100 DETA=(ETA-PSI2(N-1))/(PSI2(N)-PSI2(N-1))
100 DETA=Y/ETA
DO 125 M=2,17
125 IF(Y-PSI1(M)) 150, 150, 125
125 CONTINUE
M=17
150 DY=(Y-PSI1(M-1))/(PSI1(M)-PSI1(M-1))
200 YNM1=PSI1(M-1,N-1)+DY*(PSI1(M,N-1)-PSI1(M-1,N-1))
YN=PSI1(M-1,N)+DY*(PSI1(M,N)-PSI1(M-1,N))
250 VOIGT=YNM1+DETA*(YN-YNM1)
    IF (VOIGT-1.0) 300,251,251
251 WRITE OUTPUT TAPE 6,900
900 FORMAT(1H0, 5X, 5HVOIGT)
    WRITE OUTPUT TAPE 6,1000,VOIGT,X,ETA,DETA,DY,YNM1,YN
1000 FORMAT(1H0,2X,7E15.8)
300 RETURN
END

```

```

*   FORTRAN TALLY
*   SUBROUTINE ABSORPTION COEFFICIENT PRINTED AND WRITTEN ONTO TAPE 85- TALLY C1
C   ACCUMULATED ABSORPTION COMMON ABSMIN, TEMP, NENERGY, DENS, NSLIM, NMAX, WFACT, LTOT, K1, K2, MULT 1CT
1   IGI, NI, LI, KSI, LAI, NSI, NPI, L12I, I512I, IGF, NF, LF, KSF, MULT 2CT
2   LAF, NSF, NPI, L12F, I512F, DELTAE, Z, ALPHA, FNO, SIGSQ, GFACT, MULT 3CT
3   WCOLL, WDOPP, EI, XMCSSQ, DENMIN, NMAX, MULT 4CT
4   NOMEA, OMEGA0, DOMEA, OMEGA, ABS, AB, PSI1, PSI2, PSI MULT 1D2
DIMENSION DENS(2,6), NSLIM(6), ALPHA(6),
1   OMEGA(2000), ABS(2000,6), AB(6), PSI1(17), PSI2(8), PSI(17,8)
IF (NOMEA-2000) 50, 100, 100
50 M=NOMEA+1
DO 75 N=M, 2000
  OMEGA(N)=0.0
  DO 60 J=1,6
    60 ABS(N,J)=0.0
75 CONTINUE
100 WRITE TAPE 25, NOMEA, OMEGA0, DOMEGA, OMEGA, ABS
LC=100
200 DO 300 I=1, NOMEA
  E=8065.73*OMEGA(I)
  WAVE=12398.1/OMEGA(I)
  IF (LC-50, 250, 225
225  WRITE OUTPUT TAPE 6, 1000, TEMP, ABSMIN, NOMEA, OMEGA0, DOMEGA
  WRITE OUTPUT TAPE 6, 1020
  LC=3
250 WRITE OUTPUT TAPE 6, 1030, OMEGA(N), E, WAVE, (ABS(N,J), J=1,6)
  LC=LC+1
300 CONTINUE
  RETURN
1000 FORMAT (29H1LINE ABSORPTION COEFFICIENT-10X, 1I TEMPERATURE, 1PE12.4, TALLY F1
16H (EV.) 1PE15.4 1I 10 2E15.4 /)
1020 FORMAT (1H0, 5X, 6H ENERGY, 8X, 6H WAVE LENGTH, 26X, 32H ABSORPTION TALLY F2
1ITION COEFFICIENT (PER CM) / 1H , 6X, 4H (EV), 9X, 6H (1/CM), 6X, 10H (ANGSTTALLY F3
2ROM), 5X, 8H ALPHA(1), 6X, 8H ALPHA(2), 6X, 8H ALPHA(3), 6X, 8H ALPHA(4), 6X, 8H TALLY F4
3ALPHA(5), 6X, 8H ALPHA(6) /)
1030 FORMAT (1P9E14.4)
END

```

```

*          FORTRAN          SUBROUTINE FINIS
*          COMMON ABSMIN, TEMP, NENGY, DENS, NSLIM, NMAX, WFACT, LTOT, K1,K2, MULT 1CT
*          1  IGI, NI, LI, KSI, LAI, NSI, NPI, L12I, IS12I, IGF, NF, LF, KSF, MULT 2CT
*          2  LAF, NSF, NPF, L12F, IS12F, DELTAE, Z, ALPHA, FNO, SIGSQ, GFACT, MULT 3CT
*          3  WCOLL, WDOPP, EI, XMCSS, DENMIN, NMAX, MULT 4CT
*          4  NOMEA, OMEGA0, DOMEA, OMEGA, ABS, AB, PSI11, PSI12, PSI
*          DIMENSION DENS(2,6), NSLIM(6), ALPHA(6),
*          1  OMEGA(2000), ABS(2000,6), AB(6), PSI11(17), PSI12(8), PSI1(17,8)
*          REWIND 15
*          REWIND 25
*          CALL SFIL(15,1)
*          WRITE TAPE 15, NENGY
*          DO 100 N=1,NENGY
*          READ TAPE 25, NOMEA, OMEGA0, DOMEA, OMEGA, ABS
*          CALL MEAN
*          WRITE TAPE 15, NOMEA, OMEGA0, DOMEA, OMEGA
*          DO 50 J=1,6
*          50 WRITE TAPE 15, (ABS(N,J),N=1,2000)
*          100 CONTINUE
*          END FILE 15
*          CALL UNLOAD(15)
*          REWIND 25
*          RETURN
*          END
*          FINIS 0
*          FINIS 10
*          FINIS 20
*          FINIS 40
*          FINIS 50
*          FINIS 60
*          FINIS 70
*          FINIS 80
*          FINIS 90
*          FINIS 100
*          FINIS 120
*          FINIS 110
*          FINIS 130
*          FINIS

```

```

*          FORTRAN          MEAN          0
*          SUBROUTINE MEAN
C          CALCULATE PLANCK MEAN OPACITY MUBP
COMMON ABSMIN, TEMP, NENGY, DENS, NSLIM, NMAX, WFACT, LITOT, K1,K2,MULT 1CT
1  IGI, NI, LI, KSI, LAI, NSI, NPI, L12I, IS12I, IGF, NF, LF, KSF, MULT 2CT
2  LAF, NSF, NPF, L12F, IS12F, DELTAE, Z, ALPHA, FNO, SIGSQ, GFACT, MULT 3CT
3  WCOLL, WDOPP, EI, XMCSQ, DENMIN, NMAX, MULT 4CT
4  NOMEA, OMEGA0, DOMEGA, OMEGA, ABS, PSI1,PSI2,PSI MULT 1C2.
DIMENSION DENS(2,6),NSLIM(6),ALPHA(6),OMEGA(6),ABS(2000,6),AB(6
1)*PSI1(17)*PSI2(8),PSI(17,8)
PI=3.141592653
H=DOMEGA
T=TEMP
WRITE OUTPUT TAPE 6, 1200, OMEGA0,DOMEGA,OMEGA(NOMEA)
1200 FORMAT(42H1
1,1PE9.3,1H(,1PE9.3,1H),1PE9.3)
LINE=1
COEFF=15.0/(PI**4*T**4)
NM1=NOMEA-1
DO 500 J=1,6
N=1
AMU=ABS(N,J)
E=OMEGA(N)
F=(EXP(-E/T))*E**3*AMU
S=F
X=4.0
DO 30 N=2,NM1
AMU=ABS(N,J)
E=OMEGA(N)
F=(EXP(-E/T))*E**3*AMU
S=S+X*F
1F(X-4.0)25,20,20
20 X=2.0
GO TO 30
25 X=4.0
30 CONTINUE

```

```

N=NOMEGA
AMU=ABS(N,J)
E=OMEGA(N)
F=(EXP(F(-E/T))*E**3*AMU
S=S+F
XINT=S*H/3.0
AMUBP=COEFF*XINT
PRINT OUT
IF (LINE-50)430,410,410
410 WRITE OUTPUT TAPE 6,420
420 FORMAT(1H1)
LINE=0
430 WRITE OUTPUT TAPE 6,440,J,XINT,AMUBP
440 FORMAT(1H0,10X,3HJ= 11.5X,4HINT=1PE15.8,5X,6HAMUBP=1E15.8)
LINE=LINE+1
500 CONTINUE
RETURN
END

```

Appendix C COMPUTER CODE PIC

A brief description of the code PIC and the usage thereof is contained in this appendix. Input-output information is provided in Sec. C.1; Sec. C.2 lists the FORTRAN parameters used by the code, their definitions, and their dimensions. Section C.3 provides a brief description of each subroutine of the code, and a list of the complete source program constitutes Sec. C.4.

C.1 INPUT-OUTPUT

- A. Data cards are read in the following order (FORTRAN FORMAT in parenthesis).
 1. Card 1 - NRHO (I 10): Number of densities $N_\rho = 6$ (usually)
ALPHA0 (E 20.8): Minimum occupation α_0
TEMP (E 20.8): Temperature kT in eV
 2. Card 2 - DENS (6E 12.8): Ion densities (particles/cm³) at the 6 densities (J = 1, 6)
 3. Card 3 - EDENS (6E 12.8): Electron densities (particles/cm³) at the 6 densities (J = 1, 6)
 4. Card 4 - NEN (I 10): Number of electron energies at which the photoionization cross section is to be evaluated (≤ 50)
KHE (I 10):
$$\begin{cases} \text{KHE} = 1 \text{ oxygen} \\ \text{KHE} = 2 \text{ nitrogen} \end{cases}$$

5. Energy Cards - DELEN
(12F 6.): The electron energies (in eV) at which the photoionization cross section is to be evaluated (NEN values)

6. Card 5 - NPI (I 10): NPI = 0, Generates PHOTOIONIZATION ATLAS, continuous absorption coefficient, and Planck mean
NPI ≠ 0 is the number of cross sections in the PHOTOIONIZATION ATLAS on Tape Unit A5. Code evaluates continuous absorption coefficient and Planck mean from this atlas.

NENGY (I 10): Number of different tables of the accumulated absorption coefficient.

7. Card 6 - (Included only if NPI = 0)
NTOTAL (I 10): Number of atomic data cards.

8. NTOTAL Atomic Data Cards - (Included only if NPI = 0);
(same as for MULTIPLET, see Appendix B;
§1A3)

9. NENGY Energy Spectrum Cards - (same as for MULTIPLET, see Appendix B; §1A8)

B. The systems input tape is Tape 5; the systems output tape is Tape 6. Tape 16 (=A6) is used as a scratch tape for storage of intermediate results.

Tape 25 (=B5) contains three files of tables necessary for the calculation of the photoionization cross sections.

First file. Tables for Burgess-Seaton and hydrogenic evaluation:

NBS	(12)	Extended tables of atomic energy levels
TNBS	(1130 × 3)	
CFPO1	(2 × 6)	Tables of fractional parentage coefficients
CFPO2	(6 × 12)	
CFPO3	(12 × 20)	
CFP11	(2 × 6)	
CFP12	(6 × 12)	
CFP13	(12 × 20)	
JBS4	(4 × 4)	Burgess-Seaton tables
ABS3	(4 × 4)	
BBS3	(4 × 4)	
CBS3	(4 × 4)	
ALBS3	(4 × 4)	
BEBS3	(4 × 4)	
GBS4	(12 × 6)	
GABS5	(12 × 6)	
GBS6	(8 × 3)	
GBS7	(11 × 4)	
GBS8	(11 × 5)	
EIONK	(11)	Atomic species ionization limits
EIONE	(11)	
KLK	(10 × 5)	Hydrogenic tables
EPKL	(25)	
GAUNT	(24 × 25)	

Second and third files. Tables of parameters for analytic fit [Eq. (5.18)] to HFS bound state wave functions.

Second file: data for oxygen

ZSC	(4200)	NLSC	(620)
CSC	(4200)	KY	(620)
KX	(620)	SPEC	(8)
KTAB	(620)	NWFCTS	
IMA	(620)		

Third file. Same as second file, but data for nitrogen

Tape 15 (=A5) contains the final results of the calculation: the PHOTO-IONIZATION ATLAS and the tables of the accumulated absorption coefficients at each of the six densities - NENCY tables, one for each card $[N_{\omega}, \omega_0, \Delta\omega]$ read. The arrangement of these data on the tape follows.

• First file - PHOTOIONIZATION ATLAS

First record of first file:

NTOTAL	DELEN
ALPHAO	NRHO
TEMP	NEN

For each of the NPI photoionization cross sections there is one record (written by subroutine PTALLY):

K1	K1=0 for oxygen, K1=1 for nitrogen
K2	Charge state of atom
IGZERO	γ
NZERO	n
LZERO	l Decomposed ID of atomic state
KSZERO	$2S+1$
LAZERO	L
IBETA	β = temperature index
EKZERO	k_0 = wave number of atomic state (cm^{-1})
ALPHA	the six occupation numbers of the atomic state at the six densities being treated
CORAB	seven quantities completely specifying the given photoionization transition

OMEGAT	ω_T = photoionization threshold (eV) of the given transition
PHSIG	NEN values of the photoionization cross section - evaluated at the energies DELEN. The photoionization cross section is expressed in units of 10^{-18} cm^2 .

- Second file - The second file is organized identically to the second file of MULTIPLET Tape 15 (see Appendix B; §1B)

C. The output listing:

1. The number of photoionization transitions NPI (if NPI is initially zero).
2. The continuum absorption coefficient (cm^{-1}) for the six densities at the energies $\epsilon_N = \omega_0 + (N - 1)\Delta\omega$, ($N=1, N_\omega$)
(Written by subroutine ABRITE.)
3. The Planck mean opacity at the six densities (written by subroutine PMEAN)

Note Items 2, 3, are repeated NENGY times, once for each portion of the spectrum designated by one NENGY card.

C. 2 DEFINITIONS OF PARAMETERS IN COMMON STORAGE

Dimensions of dimensioned variables are given in parentheses.

A. PIC I and II

NOMEGA	N_ω (≤ 2000)	= Number energies in one absorption coefficient table
OMEGAO	ω_0	
DOMEGA	$\Delta\omega$	}
NRHO	N_p	= Number of densities ≤ 6 (usually set equal to 6)

ALPHA	α_0 = minimum occupation treated
TEMP	kT in eV
K1	0 for oxygen, 1 for nitrogen
K2	charge state
IGZERO	γ_0
NZERO	n_0
LZERO	l_0
KSZERO	$2s_0 + 1$
LAZERO	L_0
IBETA	β = temperature index
EZERO	E_0 = energy (eV) of given atomic state (relative to <u>neutral ground</u>)
EKZERO	k_0 = wave number of given state (relative to <u>given ground</u>)
NS	n_s = number of 2s electrons
NP	n_p = number of 2p electrons
L12	L_{12} = orbital angular momentum of core
IS12	$2s_{12} + 1$ = core spin-multiplicity
ISPEC	ISPEC = $(K_1 + K_2)$
JSPEC	JSPEC = $(6 \times K_1 + K_2)$
ZRES	Charge of residual ion = K2
ZNUCL	Nuclear charge = $(8 - K_1)$
NTOTAL	Number of atomic data cards
NIC	Number of different photoionization transitions from given initial state (≤ 10)
ZETANU	$\zeta(\nu)$ = Burgess-Seaton normalization factor
OMEGAT	ω_T = threshold photon energy (eV)
XNUI	Effective quantum number ν of Eq. (5.7)
XMUI	Quantum defect μ of Eq. (5.10)
XEPI	ϵ = electron kinetic energy (rydbergs) / $(Z_{RES})^2$

IGC	γ_c = core label of core of residual ion
NI	n_i = principal quantum number of electron being ejected
LI	l_i = orbital angular momentum of electron being ejected
ISC	$(2S_c + 1)$ = spin-multiplicity of residual ion
LC	L_c = orbital angular momentum of the residual ion
FPSQ	F_p^2 = square of fractional parentage coefficient
NEN	Number of photon energies at which cross section evaluated
NPI	Number of photoionization cross sections in atlas
NENGY	Number of tables of the absorption coefficient
DENS	(6) DENS (J) = ion density (particles/cm ³) at density J
EDENS	(6) EDENS (J) = electron density (electrons/cm ³) at density J
SLIM	(6) SLIM (J) = series limit $n_m(J)$ at density J
PIEDGE	(6) Lowering of photoionization edge at density J (eV)
ALPHA	(6) α_J = fractional occupation of state at density J
PHSIG	(50) PHSIG (N) = photoionization cross section at electron energy E_N
DELEN	(50) DELEN (N) = electron energy E_N (eV)

B. PIC I

TNBS (1130 \times 3) Data defining atomic energy levels (extended from Ref. 11)

TNBS (I, 1)	$(1000\gamma + 100l + n)$	ID of State I
TNBS (I, 2)	$(10L + (2S + 1))$	
TNBS (I, 3)	k_I = wave number (cm ⁻¹) of State I	
NBS	(12) I = NBS (J) + 1, NBS (J) + 2, ... NBS (J + 1) for Species J = JSPEC	
CFPO1	$(2 \times 6) n_s = 0, 2; n_p = 1$	Tables of the square of the fractional parentage coefficient
CFP02	$(6 \times 12) n_s = 0, 2; n_p = 2$	
CFP03	$(12 \times 20) n_s = 0, 2; n_p = 3$	
CFP11	$(2 \times 6) n_s = 1; n_p = 1$	
CFP12	$(6 \times 12) n_s = 1; n_p = 2$	
CFP13	$(12 \times 20) n_s = 1; n_p = 3$	

ABS3	$(4 \times 4) \text{ABS3}(\ell + 1, \ell' + 1) = a_{\ell\ell'}$	}	Burgess-Seaton Table III
BBS3	$(4 \times 4) \text{BBS3}(\ell + 1, \ell' + 1) = b_{\ell\ell'}$		
CBS3	$(4 \times 4) \text{CBS3}(\ell + 1, \ell' + 1) = c_{\ell\ell'}$		
ALBS3	$(4 \times 4) \text{ALBS3}(\ell + 1, \ell' + 1) = \alpha_{\ell\ell'}$		
BEBS3	$(4 \times 4) \text{BEBS3}(\ell + 1, \ell' + 1) = \beta_{\ell\ell'}$		
JBS4	$(4 \times 4) \text{Locators for Burgess-Seaton Tables IV, V}$		
	$JBS4(\ell + 1, \ell' + 1) = j(\ell, \ell')$		
	$j(0,1) = 1, j(1,0) = 2, j(1,2) = 3, j(2,1) = 4, j(2,3) = 5, j(3,2) = 6$		
GBS4	$(12 \times 6) \text{GBS4}(\nu, j) = G_{\ell\ell'}(\nu)$	Burgess-Seaton Table IV	$j = JBS4(\ell + 1, \ell' + 1)$
GABS5	$(12 \times 6) \text{GABS5}(\nu, j) = \gamma_{\ell\ell'}(\nu)$		
GBS6	$(8 \times 3) \text{GBS6}(I, 1) = G_{01}(\nu)$	Burgess-Seaton Table VI	$I = 5(\nu - 0.4) > 0$
	$GBS6(I, 2) = \gamma_{01}(\nu)$		
	$GBS6(I, 3) = \chi_{01}(\nu)$		
GBS7	$(11 \times 4) \text{GBS7}(I, 1) = G_{10}(\nu)/\sqrt{\nu - 1}$	Burgess-Seaton Table VII	$I = 5(\nu - 0.8) > 0$
	$GBS7(I, 2) = G_{10}(\nu)$		
	$GBS7(I, 3) = \gamma_{10}(\nu)$		
	$GBS7(I, 4) = \chi_{10}(\nu)$		
GBS8	$(11 \times 5) \text{GBS8}(I, 1) = G_{12}(\nu)/\sqrt{\nu - 1}$	Burgess-Seaton Table VIII	$I = 5(\nu - 0.8) > 0$
	$GBS8(I, 2) = G_{12}(\nu)$		
	$GBS8(I, 3) = \gamma_{12}(\nu)$		
	$GBS8(I, 4) = \chi_{12}(\nu)$		
	$GBS8(I, 5) = \beta_{12}(\nu)$		
EIONK	$(11) \text{EIONK}(I) = k_I$, the series limit (cm^{-1}) of Species I relative to the ground state of Species I		
EIONE	$(11) \text{EIONE}(I) = E_I$, the energy (eV) of the ground state of Species I relative to the ground state of the neutral atom		
CORE	$(7 \times 10) \text{CORE}(1, \text{IC}) = \gamma_{\text{CI}}$ core ID of initial state when <u>active</u> electron decoupled	active electron	
	$\text{CORE}(2, \text{IC}) = n_i$		
	$\text{CORE}(3, \text{IC}) = \ell_i$		

CORE (4,IC) = $2S_c + 1$, spin multiplicity of residual ion

CORE (5,IC) = L_c , orbital angular momentum of residual ion

CORE (6,IC) = F_p^2 , fractional parentage coefficient

CORE (7,IC) = k_L , ionization energy (cm^{-1}) of active electron (IC = 1,2, ..., NIC)

KLK	(10 × 5)	KLK($n, \ell + 1$) = $k_{n\ell}$, locator for Gaunt factor for initial (n, ℓ) state
EPKL	(25)	EPKL(m) = ϵ_m , energies at which Gaunt factors are tabulated
GAUNT	(24 × 25)	GAUNT($k_{n\ell}, m$) = Gaunt factor at electron energy ϵ_m for initial (n, ℓ) state
SIGHE	(50)	SIGHE(N) = high-energy approximation to the photo-ionization cross section at energy E_N = DELEN(N)
IMA	(620)	
NLSC	(620)	
KX	(620)	
NSC		
ZSC	(4200)	
CSC	(4200)	
NFUNCT		
KTAB	(620)	
NWFCTS		
KY	(620)	

} Tables for storage of parameters of HFS wave functions [Eq. (5.18)]
(See description of subroutine SLAC)

C. PIC II

OMEGA	(2000)	the photon energies at which the absorption coefficient is tabulated $\text{OMEGA}(N) = \omega_N = \omega_0 + (N - 1)\Delta\omega$, ($N = 1, N_\omega$)
PISIG	(2000)	PISIG(N) = $\sigma(\omega_N)$, the photoionization cross section at the energies ω_N ($N = 1, N_\omega$)

PIABS (2000 × 6) PIABS (N, J) = absorption coefficient (cm^{-1}) at energy ω_N , density J
CORAB (7) the quantities in array CORE for a specific transition

C.3 THE PIC FORMULA SET

Note subroutines special to nitrogen and oxygen - or atoms isoelectric thereto - are indicated by an asterisk.

A. Main Program

(Utilizes COMMON and DIMENSION of PIC-I)

1. If $\text{NPI} = 0$: PIC-I - Reads atomic data cards one at a time (NTOTAL cards in all). For each atomic state the ID is decomposed and subroutine PIENUM is called determine all the possible photoionization transitions. For each transition so determined the cross section is evaluated (subroutines PICH, PIBS, PIHE, PIACC) and written into the PHOTIONIZATION ATLAS by subroutine PTALLY.

If $\text{NPI} \neq 0$: A previously generated PHOTIONIZATION ATLAS is on Tape Unit A5. Calls PIC-II.

PIC-II (the subroutines PIABS and PFINIS): Evaluates from the PHOTIONIZATION ATLAS the continuum absorption coefficient and calculates the Planck mean opacity.

B. PIC-I

1. PISET - The initial cards are read, the line merging series limits are evaluated and the tables from Tape Unit B5 are read.
- *2. O
- *3. P
- *4. Q2
- *5. S12

*2, 3, 4, 5 } Same as MULTIPLET I

*6. PIENUM - Applies the considerations of Sec. 5 to determine all possible photoionization transitions from a given initial atomic state. For each transition determined the relevant data are stored in array CORE.

*6.1 IGAMMA - For a given species label ISPEC and given values $n_s, (2S_c + 1)$, and L_c the core labels γ_c of Table II(1) are determined. A value 9 for $(2S_c + 1)$ or L_c results in that quantity being ignored and the value of γ chosen has the smallest numerical value consistent with the remaining conditions $\neq 9$.

6.2 ESPEC - Searches TNBS for the energy of a specific state ($i, \gamma, n, \ell, L(S)$). If $S(L) = 9$, ignores $S(L)$ and accepts state of lowest energy satisfying remaining conditions on $i, \gamma, n, \ell, L(S)$. If no acceptable state is found the subroutine returns with $ESPEC = -0.0$.

*6.3 FPC - Determines the fractional parentage coefficient $FPC(n_s, n_p, S_p, L_p, S, L)$ of the decomposition

$$s^{n_s} p^{n_p} (S_L) = \sum_{S_p L_p} FPC(n_s, n_p, S_p, L_p, S, L) \left[s^{n_s} p^{n_p-1} (S_p L_p) p(S_L) \right]$$

normed $\sum_{S_p L_p} FPC = n_p$. For prohibited values of S_p, L_p , subroutine returns with $FPC = 0.0$.

7. PICH - Evaluates hydrogenic photoionization cross section at electron energies $\epsilon_N = DELEN(N), (N = 1, NEN)$

$$PHSIG(N) = \frac{107.57 \omega_T^2}{n^3 (\omega_T + \epsilon_N)^3} g_{n\ell}(\epsilon_N) \text{ FPC in terms of Gaunt factor } g_{n\ell}(\epsilon_N)$$

7.1 PGAUNT - Interpolates in table of Gaunt factors for $g_{n\ell}(\epsilon)$ at desired energy ϵ .

*8. PIBS - Evaluates Burgess-Seaton approximation to the photoionization cross section [Eq. (5.6)]. Calls BSNORM to calculate normalization

factor $\zeta(\nu)$; calls RACAH to evaluate Racah coefficient of Table I of Burgess and Seaton; calls PHASE to evaluate zero energy phase shift. Cross section evaluated in PHSIG(N) for energies $\epsilon_N = DELEN(N)$. If IBETA = 9: cross section and relevant Burgess-Seaton parameters listed.

8.1 BSNORM - Evaluates normalization factor of Eq. (5.8) according to Eq. (5.11), using the energy values tabulated in TNBS.

8.1.1 ZETA - Evaluates Eq. (5.11) for a specific atomic state.

8.1.1.1 QDE - Evaluates the quantum defect Eq. (5.10) for a specific atomic state.

8.2 RACAH - Evaluates Racah coefficient of Burgess-Seaton Table I.

8.3 PHASE - Evaluates zero-energy phase shift according to Eq. (5.12).

9. PIHE - Evaluates high-energy approximation to the photoionization cross section [Eq. (5.19)]. Calls SLAC to determine wave function of the initial bound state; function subprogram BESS to evaluate $I_\ell(\alpha, \beta)$ of Eq. (5.20). Cross section evaluated in SIGHE(N) for energies $\epsilon_N = DELEN(N)$.

If IBETA = 9: Relevant bound-state parameters listed.

9.1 SLAC - (K2, n_s, n_p, n₀, l₀, n_i, l_i; NN, ZT, CI, NBASIS) determines parameters of bound-state wave function.

$$R_{nl}(K2, n_s, n_p, n_0, l_0) = \sum_{\nu=1}^{NBASIS} C_\nu r^{\beta_\nu} \exp(-\alpha_\nu r)$$

CI(ν) = C _{ν} , ZT(ν) = α_ν , NN(ν) = β_ν (integer)

Define: IFUNCT = (10,000K₂ + 1000n_s + 100n_p + l₀) specifies the given atomic state

NOLO = (10n_i + l_i) specifies the orbital desired in the given atomic state.

KTAB(I) = IFUNCT of Ith tabulated state (determines I)

NLSC(J) = NOLO of orbital J in state I (determines J, where

KX(I) \leq J \leq [KX(I) + 9])

Then $NBASIS = IMA(J)$

$$\left. \begin{array}{l} C_\nu = CSC(L) \\ (\alpha_\nu, \beta_\nu) = ZSC(L) \end{array} \right\} KY(J) \leq L \leq [KY(J) + NBASIS]$$

(Integer β_ν in 6-low-order bits of α_ν).

9.1.1 SUBR 1, 2 - A FAP-coded subroutine to pack or unpack an integer in the 6-low-order bits of a floating number

9.2 FACTO - Evaluate $K!$ for integer K .

9.3 BESS - Evaluate $I_\ell(\alpha, \beta)$ of Eq. (5.20) according to the recursion relations Eq. (5.21).

9.3.1 BESSO - Evaluate $I_\ell(\alpha, 0)$ of Eq. (5.20), $\ell = 0, 1, 2, 3$, according to

$$I_0(\alpha, 0) = \tan^{-1}\left(\frac{1}{\alpha}\right)$$

$$I_1(\alpha, 0) = 1 - \alpha \tan^{-1}\left(\frac{1}{\alpha}\right)$$

$$I_2(\alpha, 0) = -\frac{3}{2}\alpha + \left(\frac{3}{2}\alpha^2 + \frac{1}{2}\right) \tan^{-1}\left(\frac{1}{\alpha}\right)$$

$$I_3(\alpha, 0) = \left(\frac{5}{2}\alpha^2 + \frac{2}{3}\right) - \left(\frac{5}{2}\alpha^2 + \frac{3}{2}\right)\alpha \tan^{-1}\left(\frac{1}{\alpha}\right)$$

10. PIACC - Evaluates $\sigma(\epsilon_N)$ according to Eq. (5.22) for $\epsilon_N = DELEN(N)$, ($N = 1, NEN$). To avoid the possible divergence at low energies of the high-energy approximation to the photoionization cross section. $\sigma_{HE}(\epsilon_N)$ is set equal to $\sigma_{HE}(6)$ for $N < 6$.
11. PTALLY - The contribution of a given photoionization transition is written into the PHOTOIONIZATION ATLAS on Tape A5. If IBETA = 9, the cross section and relevant parameters are listed.

C. PIC-II

1. PIABS - For each table of the absorption coefficient (NENGY tables in all): the photoionization transitions are read from the PHOTOIONIZATION ATLAS one at a time and the photoelectric absorption coefficient is

accumulated for each density J at all photon energies greater than $[\omega_T - \text{PIEDGE}(J)]$, the lowered photoelectric edge at density J . Calls **ABRITE**.

1. 1 **ABRITE** – Absorption coefficient table written onto Tape A6 and listed.
2. **PFINIS** – Transfers absorption coefficient tables from Tape A6 to the second file of Tape A5. Calls **PMEAN**.
2. 1 **PMEAN** – Evaluates and lists the photoelectric contribution to the Planck mean opacity – by numerical integration of the tabulated absorption coefficient for each of the **NENGY** tables.

C.4 LIST OF SOURCE PROGRAM OF PIC

```

0
* FORTRAN
  PIC- MAIN PROGRAM
  COMMON NOMEGA, OMEGA0, DOMEGA, NRHO, ALPHAO, TEMP, K1, K2, IGZERO, PICCOMM1
1  NZERO, LZERO, KZERO, LAZERO, IBETA, EZERO, EKZERO, NS, NP, L12, PICCOMM2
2  IS12, ISPEC, JSPEC, ZRES, ZNUCL, NTOTAL, NIC, ZETANU, OMEGAT, PICCOMM3
3  XNUJI, XMUI, XEPI, IGC, NI, LI, ISC, LC, FPSQ, NEN, NPI, NENGY, PICCOM 4
4  DENS, EDENS, SLIM, PIEDGE, ALPHA, PHSIG, DELEN, PICCOM 5
5  TNBS, NBBS, CFP01, CFP02, CFP03, CFP11, CFP12, CFP13, ABS3, BBS3, CBS3, ALBS3, PICCOM16
6  BEBS3, JBS4, GBS4, GBS5, GBS6, GBS7, EIONK, EIONE, CORE, KLK, EPKL, PICCOM17
7  GAUNT, SIGHE, IMA, NLSC, KX, NSC, ZSC, CSC, NFUNCT, KTAB, NWFCTS, KY PICCOM18
  DIMENSION DENS(6), EDENS(6), SLIM(6), PIEDGE(6), ALPHA(6), PICDIM 1
1  PHSIG(50), DELEN(50), PICDIM 2
2  TNBS(1130,3), NBS(12), CFP01(2,6), CFP02(6,12), CFP03(12,20), PICDIM13
3  CFP11(2,6), CFP12(6,12), CFP13(12,20), ABS3(4,4), BBS3(4,4), PICDIM14
4  CBS3(4,4), ALBS3(4,4), BEBS3(4,4), JBS4(4,4), GBS4(12,6), PICDIM15
5  GBS5(12,6), GBS6(8,3), GBS7(11,4), GBS8(11,5), EIONK(11), PICDIM16
6  EIONE(11), CORE(7,10), KLK(10,5), EPKL(25), GAUNT(24,25), PICDIM17
7  SIGHE(50), ZSC(4200), CSC(4200), KX(620), KTAB(620), PICDIM18
8  IMA(620), NLSC(620), KY(620), NN(20), ZT(20), CI(20), SPEC(8), PICDIM19
  CALL PISET
  READ INPUT TAPE 5, 1000, NPI, NENGY
  IF(INPI) 10, 600
10  READ INPUT TAPE 5, 1010, NTOTAL
20  WRITE TAPE 15, NTOTAL, ALPHAO, TEMP, DELEN, NRHO, NEN
  DO 500 NCASE=1,NTOTAL
30  READ INPUT TAPE 5, 1020, K1, K2, IGZERO, NZERO, LZERO, KSZERO,
1  LAZERO, IBETA, EZERO, ALPHA
  DO 40 J=1,NRHO
    IF(ALPHA(J)-ALPHAO) 40, 50, 50
40  CONTINUE
  GO TO 500
50  JSPEC=6*K1+K2
    ISPEC=K1+K2
    ZRES=K2
    ZNUCL=8-K1
    EKZERO=8065.98*(EZERO-EIONE (JSPEC))

```

```

70 NS=0(K1, K2, IGZERO, NZERO, LZERO, KSZERO, LAZERO)
NP=P(K1, K2, IGZERO, NZERO, LZERO, KSZERO, LAZERO)
L12=Q2(K1, K2, IGZERO, NZERO, LZERO, KSZERO, LAZERO)
IS12=2.0*S12(K1, K2, IGZERO, NZERO, LZERO, KSZERO, LAZERO)+1.0
100 CALL PIENUM
    IF(INIC-10) 115, 110
110 WRITE OUTPUT TAPE 6, 1030, K1, K2, IGZERO, NZERO, LZERO, KSZERO,
1    LAZERO, NIC, CORE
    GO TO 500
115 IF(INIC)110, 110, 120
120 DO 300 IC=1, NIC
    IF(ICORE(7,IC)) 125, 125, 130
125 WRITE OUTPUT TAPE 6, 1030, K1, K2, IGZERO, NZERO, LZERO, KSZERO,
1    LAZERO, NIC, CORE
    GO TO 300
130 OMEGAT=(CORE(7,IC)-EKZERO)/8065.98
    DO 140 N=1.50
    PHSIG(N)=0.0
140 SIGHE(N)=0.0
    IF(ICORE(2,IC)-6.0)160, 150, 150
150 CALL PICH(IC)
    GO TO 200
160 IF(ICORE(3,IC)-2.0) 170, 150, 150
170 CALL PIBS(IC)
180 CALL PIHE(IC)
190 CALL PIACC
200 CALL PTALLY(IC)
200 CONTINUE
500 CONTINUE
    END FILE 15
    REWIND 15
    WRITE OUTPUT TAPE 6, 1040, NPI
600 CALL PIABS
700 CALL PFINIS
    CALL EXIT
1000 FORMAT(2I10)

```

```
1010 FORMAT(I10)          F2
1020 FORMAT(2I1,2I2,4I1,E10.8,6E8.6)   F3
1030 FORMAT(7H1ERROR-2I1,2I2,4I1/(6E20.8)) F4
1040 FORMAT(48H1NUMBER OF PHOTOIONIZATION TRANSITIONS IN 'ATLAS',I5) F5
END          PIC
```

```

*          FORTRAN          0
*          SUBROUTINE PISET          0
*          SET UP PHOTOIONIZATION CALCULATION-
*          COMMON NOMEGA, OMEGA0, DOMEGA, NRHO, ALPHA0, TEMP, K1, K2, IGZERO, PICCOMM1
*          1  NZERO, LZERO, KSZERO, LAZERO, IBETA, EZERO, EKZERO, NS, NP, L12, PICCOMM2
*          2  IS12, ISPEC, ZRES, ZNUCL, NTOTAL, NIC, ZETANU, OMEGAT, PICCOMM3
*          3  XNU1, XMUI, XEPI, IGC, NI, LI, ISC, LC, FPSQ, NEN, NPI, NENY,
*          4  DENS, EDENS, SLIM, PIEDGE, ALPHA, PHSIG, DELEN, PICCOM 4
*          5  TNBS, NBS, CFP01, CFP02, CFP03, CFP11, CFP12, CFP13, ABS3, BBS3, CBS3, ALBS3, PICCOM16
*          6  BEBS3, JBS4, GBS4, GABSS, GBS6, GBS7, GBS8, EIONK, EIONE, CORE, KLK, EPKL, PICCOM17
*          7  GAUNT, SIGHE, IMA, NLSC, KX, NSC, ZSC, CSC, NFUNCT, KTAB, NWFCTS, KY
*          DIMENSION DENS(6), EDENS(6), SLIM(6), PIEDGE(6), ALPHA(6), PICDIM 1
*          PHSIG(50), DELEN(50), PICDIM 2
*          1  TNBS(1130,3), NBS(12), CFP01(2,6), CFP02(6,12), CFP03(12,20), PICDIM13
*          2  CFP11(2,6), CFP12(6,12), CFP13(12,20), ABS3(4,4), BBS3(4,4), PICDIM14
*          3  CBS3(4,4), ALBS3(4,4), BEBS3(4,4), JBS4(4,4), GBS4(12,6), PICDIM15
*          4  GABSS(12,6), GBS6(8,3), GBS7(11,4), GBS8(11,5), EIONK(11), PICDIM16
*          5  EIONE(11), CORE(7,10), KLK(10,5), EPKL(25), GAUNT(24,25), PICDIM17
*          6  SIGHE(50), ZSC(4200), CSC(4200), KX(620), KTAB(620), PICDIM18
*          7  IMA(620), NLSC(620), KY(620), NN(20), ZT(20), CI(20), SPEC(8), PICDIM19
*          8  PISET 10
*          REWIND 15
*          REWIND 16
*          REWIND 25
*          READ INPUT TAPE 5, 1000, NRHO, ALPHA0, TEMP, DENS, EDENS, PISET 30
*          WRITE OUTPUT TAPE 6, 1010, TEMP, (DENS(J), EDENS(J), J=1, NRHO)
*          DO 50 J=1, NRHO
*          IF (EDENS(J)) 50, 50, 20
*          20  SLIM(J)=(4.107E22*SORTF(TEMP)/EDENS(J))** (1.7)
*          IF (SLIM(J)-7.0) 30, 50, 50
*          30  SLIM(J)=7.0
*          50  CONTINUE
*          READ TAPE 25, NBS, TNBS, CFP01, CFP02, CFP11, CFP12, PISET100
*          1  CFP13, JBS4, ABS3, BBS3, CBS3, ALBS3, BEBS3, GBS4, GABSS, GBS6, PISET110
*          2  GBS7, GBS8, EIONK, EIONE, KLK, EPKL, GAUNT, PISET120
*          PISET130
*          PISET140
*          REWIND 25
*          READ INPUT TAPE 5, 1020, NEN, KHE
*          100 READ INPUT TAPE 5, 1020, NEN, KHE

```



```

*   FORTRAN
*   FUNCTION O(I1,I2,I3,I4,I5,I6,I7)
C   COMPUTES NUMBER OF ELECTRONS IN THE 2S SHELL
I=I1+I2
IG=I3
      GO TO (8,9,10,11,12,13),I
      8 GO TO(3,3,3,2,2,2,1),IG
      9 GO TO(3,3,3,2,2,2,1,1),IG
      10 GO TO(3,2,2,2,2,1,1),IG
      11 GO TO(3,2,2,1,1,1),IG
      12 GO TO (2,1),IG
      13 IF((I4-2)14,14,1
      14 IL=1+17
      GO TO(2,1),IL
      15 IF((I4+IG+17-3)3,3,16
      1 O=0.0
      2 RETURN
      2 O=1.0
      3 RETURN
      3 O=2.0
      RETURN
      END

```

```

*   FORTRAN
*   FUNCTION P(I1,I2,I3,I4,I5,I6,I7)
C   COMPUTES NUMBER OF ELECTRONS IN THE 2P SHELL
I3=13
I=I1+I2
GO TO (8,9,10,11,12,13),I
8 GO TO(4,4,4,5,5,5,6),IG
9 GO TO(3,3,4,4,4,4,5,5,5),IG
10 GO TO(2,3,3,3,4,4,4),IG
11 GO TO(1,2,2,3,3,3),IG
12 IF (I4+IG+17-3)15,15,16
13 IF (I4-2)14,14,1
14 IL=1+17
GO TO(15,1),IL
15 P=0.0
RETURN
16 GO TO(1,2),IG
1 P=0.0
22 IF (I4-2)20,21,20
2 P=1.0
GO TO 22
3 P=2.0
4 GO TO 22
4 P=3.0
5 GO TO 22
5 P=4.0
6 GO TO 22
6 P=5.0
GO TO 22
21 P=P+1.0
20 RETURN
END

```

```

* FORTRAN          FUNCTION L2 CALLED Q2.
C
FUNCTION Q2(I1,I2,I3,I4,I5,I6,I7)
IF(I4-2)200,100,200
100 Q2=17
RETURN
200 I=I1+I2
      GO TO (1,2,3,4,5,6),I
1   GO TO (6,8,7,7,8,6,7,7),I3
2   GO TO (7,8,6,6,8,7,8,6,7,7,8,6),I3
3   GO TO (7,7,8,6,7,6,8,7),I3
4   GO TO (6,7,7,7,8,6),I3
5   GO TO (6,7),I3
6   Q2=0.
      RETURN
7   Q2=1.
      RETURN
8   Q2=2.
      RETURN
END

```

```

*      FORTRAN
      FUNCTION S12(I1,I2,I3,I4,I5,I6,I7)
      IF(I4-2)100,100,200
100   S12=16
      S12=(S12-1.*1/2.
      RETURN
200   I=I1+I2
      GO TO (1,2,3,4,5,6),I
1     GO TO (7,8,8,7,8,8,8),I3
2     GO TO (9,6,6,10,9,9,6,9,6,9,6,6),I3
3     GO TO (8,7,8,8,8,7,8,8),I3
4     GO TO (6,9,6,9,6,6),I3
5     GO TO (8,8),I3
6     S12=0.
      RETURN
7     S12=1.*5
      RETURN
8     S12=.5
      RETURN
9     S12=1.
      RETURN
10    S12=2.
      RETURN
      END

```

```

* FORTRAN
* SUBROUTINE PIENUM
* ENUMERATES FINAL STATES
* COMMON NOMEGA, OMEGA0, DOMEGA, NRHO, ALPHAO, TEMP, K1, K2, IGZERO, PICCOMM1
* 1 NZERO, LZERO, KSZERO, LAZERO, IBETA, EZERO, EKZERO, NS, NP, L12, PICCOMM2
* 2 IS12, ISPEC, JSPEC, ZRES, ZNUCL, NTOTAL, NIC, ZETANU, OMEGAT, PICCOMM3
* 3 XNUI, XMUI, XEPI, IGC, NI, LI, ISC, LC, FPSQ, NEN, NPI, NENGY, PICCOM 4
* 4 DENS, EDENS, SLIM, PIEDGE, ALPHA, PHSIG, DELEN, PICCOM 5
* 5 TNBS, NBS, CFP01, CFP02, CFP03, CFP11, CFP12, CFP13, ABS3, BBS3, CBS3, ALBS3, PICCOM16
* 6 BEBS3, JBS4, GBS4, GABS5, GBS6, GBS7, GBS8, EIONK, EIONE, CORE, KLK, EPKL, PICCOM17
* 7 GAUNT, SIGHE, IMA, NLSCL, NSC, ZSC, CSC, NFUNCT, KTAB, NWFCTS, KY
* DIMENSION DENS(6), EDENS(6), SLIM(6), PIEDGE(6), ALPHA(6), PICDIM 1
* 1 PHSIG(50), DELEN(50), PICDIM 2
* 2 TNBS(1130,3), NBS(12), CFP01(2,6), CFP02(6,12), CFP03(12,20), PICDIM13
* 3 CFP11(2,6), CFP12(6,12), CFP13(12,20), ABS3(4,4), BBS3(4,4), PICDIM14
* 4 CBS3(4,4), ALBS3(4,4), BEBS3(4,4), JBS4(4,4), GBS4(12,6), PICDIM15
* 5 GABS5(12,6), GBS6(8,3), GBS7(11,4), GBS8(11,5), EIONK(11), PICDIM16
* 6 EIONE(11), CORE(7,10), KLK(10,5), EPKL(25), GAUNT(24,25),
* 7 SIGHE(50),
* 8 IMA(620), NLSCL(620), KY(620), NN(20), ZT(20), CI(20), SPEC(8), PICDIM18
* IC=0
* 1 IF(IZERO-2)400, 50, 10
* 10 IC=IC+1
* CORE(1,IC)=IGZERO
* CORE(2,IC)=NZERO
* CORE(3,IC)=LZERO
* CORE(4,IC)=IS12
* CORE(5,IC)=L12
* CORE(6,IC)=1.0
* IGCf=IGAMMA(JSPEC+1, NS, 9.9)
* IF(INP) 12, 12, 14
* 12 LPP=0
* GO TO 15
* 14 LPP=1
* 15 CORE(7,IC)=EIONK(JSPEC)+ESPEC(K1, K2+1, IGCf, 2, LPP, IS12, L12)
* 50 IF(INP) 220, 220, 60
* PIENUM 0
* PIENUM1
* PIENUM2
* PIENUM3
* PIENUM4
* PIENUM5
* PIENUM6
* PIENUM7
* PIENUM8
* PIENUM9
* PIENUM10
* PIENUM11
* PIENUM12
* PIENUM13
* PIENUM14
* PIENUM15
* PIENUM16

```

```

60 DO 210 I=1,3,2
70 DO 200 J=1,3
    ISP=IS12-2+I
    LP=L12+J-2
    X=FPC(NS, NP, ISP, LP, IS12, L12)
    IF(X) 80,200, 80
80  IC=IC+1
    CORE(2,IC)=2
    CORE(3,IC)=1
    CORE(6,IC)=X
    IF(NZERO-2)130, 100, 130
100 IF(NP-1) 110, 110, 115
110 LPP=0
    GO TO 120
115 LPP=1
120 ISC=ISP
    LC=LP
    IGCF=IGAMMA(ISPEC+1, NS, 9,9)
    GO TO 150
130 ISC=9
    LC=9
    IGCF=IGAMMA((ISPEC+1,NS,ISP, LP)
    LPP=LZERO
150 CORE(1,IC)=IGAMMA(ISPEC, NS, ISC, LC)
    CORE(4,IC)=ISC
    CORE(5,IC)=LC
    Y=ESPEC(K1,K2+1,IGCF,NZERO,LPP,ISC,LC)
    IF(Y) 155, 160, 160
155 ITAG=0
    GO TO 500
160 CORE(7,IC)=EIONK(JSPEC)+Y
200 CONTINUE
210 CONTINUE
220 IF(NS) 230, 230, 250
230 GO TO 390
250 IF(NZERO-2)300, 260, 300

```

```

260 IF(NP)300, 270, 300
270 IC=IC+1
  CORE(1,IC)=IGAMMA(ISPEC,NS-1,NS,0)
  CORE(2,IC)=2
  CORE(3,IC)=0
  CORE(4,IC)=NS
  CORE(5,IC)=0
  CORE(6,IC)=NS
  CORE(7,IC)=EIONK(JSPEC)+ESPEC(K1, K2+1,IGCF, 2, 0, NS, 0)
GO 10 390
300 DO 370 I=1, 3, 2
  ISP=IS12-2+1
  IF(ISP-1)370, 302, 302
  IF(INZERO-2)330, 320, 330
  302 IF(ISP-NS-NP)305, 305, 370
  303 IF(ISP-NS-NP-1)305, 305, 370
  304 IF(ISP-NS-NP-1)305, 305, 370
  305 IG=IGAMMA(ISPEC, NS-1, ISC, LC)
  IF(NS-1)307, 307, 310
  307 X=1.0
  IF(IG)370, 370, 315
  310 X=FLOATF(ISP)/FLOATF(IS12)
  315 IC=IC+1
  CORE(2,IC)=2
  CORE(3,IC)=0
  CORE(6,IC)=X
  LPP=LZERO
  GO 10 350
  320 ISC=ISP
  LC=L12
  IGCIF=IGAMMA(ISPEC+1,NS-1, 9,9)
  GO 10 303
  330 ISC=9
  LC=9
  IGCIF=IGAMMA(ISPEC+1,NS-1, ISP, L12)
  IF(IGCF)370, 370, 304
  PIEN A74

```

```

350 CORE(1,IC)=IG
  CORE(4,IC)=ISC
  CORE(5,IC)=LC
  Y=ESPEC(K1,K2+1,IGCF,NZERO,LZERO,ISC,LC)
  IF(Y) 355, 360
  355 ITAG=1
    GO TO 500
  360 CORE(7,IC)=EIONK(JSPEC)+Y
  365 IF(NS-1) 390, 370
  370 CONTINUE
  390 NIC=IC
    RETURN
  400 NIC=0
    RETURN
  500 IF(NZERO-3) 510, 530, 600
  510 Y=ESPEC(K1,K2+1,IGCF,NZERO,LPP,9,LC)
    IF(Y) 520, 550
  520 Y=ESPEC(K1, K2+1,IGCF,NZERO,LPP,9,9)
    IF(Y) 530, 550, 550
  530 Y=-1.0E+8
  550 IF(ITAG) 360, 160, 360
  600 LPP=XMINOF(LPP,2)
    YP=ESPEC(K1,K2+1,IGCF,3,LPP,9,9)
    IF(YP) 530, 610, 610
  610 Y=ESPEC(K1, K2,IGZERO,3,LPP,9,9)
    IF(Y) 530, 620, 620
  620 Y=EKZERO+YP-Y
    GO TO 550
  END

```

```

*      FORTRAN
*      LIST
      FUNCTION IGAMMA(I,NS,IS,L)
      IF(I-6)300,300,200
      200  IGAMMA=0
      RETURN
      300  NSP1=NS+1
            LP1=L+1
            GO TO (1,36,75,104,131,144),I
      1  GO TO (2,13,25),NSP1
      2  IF (IS-9)3,4,4
      3  GO TO (5,4,5,5,5),IS
      4  IF (L-9)7,10,10
      5  IGAMMA=0
      RETURN
      7  GO TO (8,10,8),LP1
      8  IGAMMA=0
      RETURN
      10  IGAMMA=6
      RETURN
      13  IF (IS-9)14,23,23
      14  IF (L-9)15,22,22
      15  GO TO (5,16,5,20,5),IS
      16  GO TO (17,18,19),LP1
      17  IGAMMA=6
      RETURN
      18  IGAMMA=7
      RETURN
      19  IGAMMA=5
      RETURN
      20  GO TO (8,21,8),LP1
      21  IGAMMA=4
      RETURN
      22  GO TO (5,19,5,21,5),IS
      23  IF (L-9)24,21,21
            +      00000020
            00000030
            10
            20
            30
            40
            50
            60
            70
            80
            90
            100
            110
            120
            130
            140
            150
            160
            170
            180
            190
            200
            210
            220
            230
            240
            250
            260
            270
            280
            290
            300
            310
            320
            330
            340

```

```

24 GO TO(17,21,19),LP1
25 IF(15-9)26,34,34
26 IF(L-9)27,33,33
27 GO TO(5,28,5,31,5),IS
28 GO TO(8,29,30),LP1
29 1GAMMA=3
      RETURN
30 1GAMMA=2
      RETURN
31 GO TO(32,8,8),LP1
32 1GAMMA=1
      RETURN
33 GO TO(5,30,5,32,5),IS
34 IF(L-9)35,32,32
35 GO TO(32,29,30),LP1
36 GO TO(37,48,64),NSP1
37 IF(15-9)38,46,46
38 IF(L-9)39,45,45
39 GO TO(40,5,43,5,5),IS
40 GO TO(41,8,42),LP1
41 1GAMMA=12
      RETURN
42 1GAMMA=11
      RETURN
43 GO TO(8,44,8),LP1
44 1GAMMA=10
      RETURN
45 GO TO(42,5,44,5,5),IS
46 IF(L-9)47,44,44
47 GO TO(41,44,42),LP1
48 IF(15-9)49,61,61
49 IF(L-9)50,60,60
50 GO TO(51,5,54,5,58),IS
51 GO TO(8,52,53),LP1
52 1GAMMA=9
      RETURN

```

```

53 1GAMMA=7
  RETURN
54 GO TO(55,56,57),LP1
55 1GAMMA=8
  RETURN
56 1GAMMA=6
  RETURN
57 1GAMMA=5
  RETURN
58 GO TO(59,6,8),LP1
59 1GAMMA=4
  RETURN
60 GO TO (53,5,57,5,59),IS
61 IF(L-9)62,59,59
62 GO TO(59,56,57),LP1
63 IF (IS-9)65,73,73
64 IF (L-9)66,72,72
65 GO TO(67,5,70,5,5),IS
66 GO TO(68,8,69),LP1
67 GO TO(68,8,69),LP1
68 1GAMMA=3
  RETURN
69 1GAMMA=2
  RETURN
70 GO TO(8,71,8),LP1
71 1GAMMA=1
  RETURN
72 GO TO(69,5,71,5,5),IS
73 IF(L-9) 74,71,71
74 GO TO (68,71,69),LP1
75 GO TO(76,87,99),NSP1
76 IF (IS-9)77,85,85
77 IF (L-9)78,84,84
78 GO TO( 5,79, 5,82, 5),IS
79 GO TO( 8,80,81),LP1
80 1GAMMA=8
  RETURN

```

```

81 1GAMMA=7
    RETURN
82 GO TO(83,8,8),LP1
83 1GAMMA=6
    RETURN
84 GO TO(5,81,5,83),IS
85 IF(L-9)86,83,83
86 GO TO(83,80,81),LP1
87 IF(IS-9)88,97,97
88 IF(L-9)89,96,96
89 GO TO(5,90,5,94,5),IS
90 GO TO(91,92,93),LP1
91 1GAMMA=4
    RETURN
92 1GAMMA=5
    RETURN
93 1GAMMA=3
    RETURN
94 GO TO(8,95,8),LP1
95 1GAMMA=2
    RETURN
96 GO TO(5,93,5,95,5),IS
97 IF(L-9)98,95,95
98 GO TO(91,95,93),LP1
99 IF(IS-9)100,101,101
100 GO TO(5,101,5,5,5),IS
101 IF(L-9)102,103,103
102 GO TO(8,103,8),LP1
103 1GAMMA=1
    RETURN
104 GO TO(105,116,126),NSP1
105 IF(IS-9)106,114,114
106 IF(L-9)107,113,113
107 GO TO(108,5,111,5,5),IS
108 GO TO(109,8,110),LP1
109 1GAMMA=6

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      RETURN
110 1GAMMA=5
      RETURN
111 GO TO(8,112,8),LP1
112 1GAMMA=4
      RETURN
113 GO TO(110,5,112,5,5),IS
114 IF(L-9)115,112,112
115 GO TO(109,112,110),LP1
116 IF(15-9)117,124,124
117 IF(L-9)118,123,123
118 GO TO(119,5,121,5,5),IS
119 GO TO(8,120,8),LP1
120 1GAMMA=3
      RETURN
121 GO TO(8,122,8),LP1
122 1GAMMA=2
      RETURN
123 GO TO(120,5,122,5,5),IS
124 IF(L-9)125,122,122
125 GO TO(8,122,8),LP1
126 IF(15-9)127,128,128
127 GO TO(128,5,5,5,5),IS
128 IF(L-9)129,130,130
129 GO TO(130,8,8),LP1
130 1GAMMA=1
      RETURN
131 GO TO(134,139,139),NSP1
132 WRITE OUTPUT TAPE 6,133,NS
133 FORMAT(1H0,3X,17HERROR IN NS)
134 IF(15-9)135,136,136
135 GO TO(5,136,5,5,5),IS
136 IF(L-9)137,138,138
137 GO TO(8,138,8),LP1

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138 IGAMMA=2
139 RETURN
140 IF (IS-9)140,141,141
141 GO TO (5,141,5,5,5),IS
142 IF (L-9)142,143,143
143 GO TO (143,8,8),LP1
144 IGAMMA=1
145 RETURN
146 GO TO (145,145,132),NSP1
147 IF (IS-9)146,147,147
148 GO TO (147,5,5,5,5),IS
149 IF (L-9)148,149,149
150 GO TO (149,8,8),LP1
151 IGAMMA=1
152 RETURN
153 END
```

```

*   FORTRAN ESPEC(IX1,IX2,IGAM, N, L, ISBAR, LTOT)
COMMON NOMEA, OMEAO, DOMEA, NRHO, ALPHA0, TEMP, K1, K2, IGZERO, PICCOMM1
1  NZERO, LZERO, KSZERO, LAZERO, IBETA, EZERO, EKZERO, NS, NP, L12, PICCOMM2
2  IS12, ISPEC, JSPEC, ZRES, ZNUCL, NTOTAL, NIC, ZETANU, OMEGAT, PICCOMM3
3  XNUI, XMUI, XEPI, IGC, NI, LI, ISC, LC, FPSQ, NEN, NPI, NENY,
4  DENS, EDENS, SLIM, PLEDGE, ALPHA, PHSIG, DELEN, PICCOM 4
5  TNBS, NBS, CFP01, CFP02, CFP03, CFP11, CFP12, ABS3, BBS3, CBS3, ABS3, PICCOM 5
6  BEBS3, JBS4, GBS5, GBS6, GBS7, GBS8, EIONK, EIONE, CORE, KLK, EPKL, PICCOM17
7  GAUNT, SIGHE, IMA, NLSC, KX, NSC, ZSC, CSC, NFUNC, KTAB, NWFCTS, KY
DIMENSION DENS(6), EDENS(6), SLIM(6), PLEDGE(6), ALPHA(6),
PHSIG(50), DELEN(50),
1  TNBS(1130,3), NBS(12), CFP01(2,6), CFP02(6,12), CFP03(12,20),
2  CFP11(2,6), CFP12(6,12), CFP13(12,20), ABS3(4,4), BBS3(4,4),
3  CBS3(4,4), ALBS3(4,4), BEBS3(4,4), JBS4(4,4), GBS4(12,6),
4  GBS5(12,6), GBS6(8,3), GBS7(11,4), GBS8(11,5), EIONK(11),
5  EIONE(11), CORE(7,10), KLK(10,5), EPKL(25), GAUNT(24,25),
6  SIGHE(50),
7  ZSC(4200), CSC(4200), KX(620), KTAB(620),
8  IMA(620), NLSC(620), KY(620), NN(20), ZT(20), SPEC(8),
9  IF(IX1+IX2-6) 20, 20, 10
10  ESPEC=0.0
      RETURN
20  J=6#IX1+IX2
    IL=NBS(J)+1
    IM=NBS(J+1)
    X=1000*IGAM+100*L+N
    DO 100  I=IL,IM
      IF(X-TNBS(I,1)) 100, 25, 100
    100  LNBS=TNBS(I,2)/10.0
25  ISNBS=TNBS(I,2)-10.0*FLOATF(LNBS)
    IF(LTOT-9) 30, 35, 30
    30  IF(LTOT-LNBS) 100, 35, 100
    35  IF(ISBAR-9) 40, 45, 40
    40  IF(ISBAR-ISNBS) 100, 45, 100
    45  ESPEC=ABSF(ITNBS(I,3))
      RETURN

```

100 CONTINUE
ESPEC=-1.0E-5
RETURN
END

ESPEC 18
ESPEC 19
ESPEC 20
ESPEC

```

* FORTRAN
FUNCTION FPC(I, J, IXP, IYP, IX, IY)
COMMON NOMEA, OMEGA0, DOMEGA, NRHO, ALPHAO, TEMP, K1, K2, IZERO, PICCOMM1
1 NZERO, LZERO, KSZERO, LAZERO, IBETA, EZERO, EKZERO, NS, NP, L12, PICCOMM2
2 IS12, ISPEC, JSPEC, ZRES, ZNUCL, NTOTAL, NIC, ZETANU, OMEGAT, PICCOMM3
3 XNU1, XMUI, XEP1, IGC, NI, LI, ISC, LC, FPSQ, NEN, NPI, NENY,
4 DENS, EDENS, SLIM, PIEDGE, ALPHA, PHSIG, DELEN, PICCOMM4
5 TNBS, NBS, CFP01, CFP02, CFP03, CFP11, CFP12, CFP13, ABS3, BBS3, CBS3, ALBS3, PICCOMM5
6 BEBS3, JBS4, GBS4, GABSS5, GBS6, GBS7, GBS8, EIONK, EIONE, CORE, KLK, EPKL, PICCOMM17
7 GAUNT, SIGHE, IMA, NLSC, KX, NSC, ZSC, CSC, NFUNC, KTAB, NWFCTS, KY
DIMENSION DENS(6), EDENS(6), SLIM(6), PIEDGE(6), ALPHA(6),
1 PHSIG(50), DELEN(50), PICDIM1
2 TNBS(1130, 3), NBS(12), CBS01(2, 6), CFP01(2, 6), CFP02(6, 12), CFP03(12, 20),
3 CFP11(2, 6), CFP12(6, 12), CFP13(12, 20), ABS3(4, 4), BBS3(4, 4), PICDIM13
4 CBS3(4, 4), ALBS3(4, 4), BEBS3(4, 4), JBS4(4, 4), GBS4(12, 6), PICDIM14
5 GABSS5(12, 6), GBS6(8, 3), GBS7(11, 4), GBS8(11, 5), EIONK(11), PICDIM15
6 EIONE(11), CORE(7, 10), KLK(10, 5), EPKL(25), GAUNT(24, 25), PICDIM16
7 SIGHE(50),
8 IMA(620), NLSC(620), KY(620), NN(20), ZT(20), CI(20), SPEC(8),
1 IF( J) 10, 10, 20, PICDIM19
10 FPC=0.0
      RETURN
20 IF(IY)100, 22, 22, FPC 1
22 IF(IY-J) 24, 24, 100, FPC 2
24 IF(IX-1)100, 26, 26, FPC 3
26 IF(IX-J-2) 40, 40, 100, FPC 4
30 IF(IYP) 10, 32, 32, FPC 5
32 IF(IYP-J+1) 34, 34, 10, FPC 6
34 IF(IXP-1) 10, 36, 36, FPC 7
36 IF(IXP-J-1) 70, 70, 10, FPC 8
40 IF(J-3) 50, 50, 60, FPC 9
50 FPC=1.0, FPC 10
      K=(J+2)*IY+IX, FPC 11
      KP=(J+1)*IYP+IXP, FPC 12
      JP=J, FPC 13
      GO TO 30, FPC 14
      FPC 15
      A15, FPC 16

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60 FPC=FLOATF(IXP*(2*IY+1))/FLOATF(IX*(2*IY+1))
JP=7-J
K=(JP+2)*IY+IXP
KP=(JP+1)*IY+IX
GO TO 30
70 IF(I--1) 80, 90, 80
80 GO TO (82, 84, 86),JP
82 FPC=FPC*CFP01(KP,K)
RETURN
84 FPC=FPC*CFP02(KP,K)
RETURN
86 FPC=FPC*CFP03(KP,K)
RETURN
90 GO TO (92, 94, 96),JP
92 FPC=FPC*CFP11(KP,K)
RETURN
94 FPC=FPC*CFP12(KP,K)
RETURN
96 FPC=FPC*CFP13(KP,K)
RETURN
100 WRITE OUTPUT TAPE 6, 150, I, J, IXP, IY, IX, IY
GO TO 10
150 FORMAT(10H1FPC ERROR10X6I10)
END

```

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*          FORTRAN          PICH 0
*          SUBROUTINE PICH(K)          PICH 0
*          EVALUATES HYDROGENIC PHOTIONIZATION FOR KTH CORE          PICH C1
*          COMMON NOMEGA, OMEGA0, DOMEGA, NRHO, ALPHA0, TEMP, K1, K2, IGZERO, PICCOMM1
*          NZERO, LZERO, KSZERO, LAZERO, IBETA, EZERO, EKZERO, NS, NP, L12, PICCOMM2
*          IS12, ISPEC, JSPEC, ZRES, ZNUCL, NTOTAL, NIC, ZETANU, OMEGAT, PICCOMM3
*          3XNUI, XMUI, XEPI, IGC, NI, LI, ISC, LC, FPSQ, NEN, NPI, NENGY, PICCOM 4
*          4DENS, EDENS, SLIM, PIEDGE, ALPHA, PHSIG, DELEN, PICCOM 5
*          STNBS, NBS, CFP01, CFP02, CFP03, CFP11, CFP12, CFP13, ABS3, BBS3, CBS3, ALBS3, PICCOM16
*          6BEBS3, JBS4, GBS4, GAB55, GBS6, GBS7, EIONK, EICNE, CORE, KLK, EPKL, PICCOM17
*          7GAUNT, SIGHE, IMA, NLSC, KX, NSC, ZSC, CSC, NFUNCT, KTAB, NWFCTS, KY PICCOM18
*          PICDIM 1
*          DIMENSION DENS(6), EDENS(6), SLIM(6), PIEDGE(6), ALPHA(6), PICDIM 2
*          PHSIG(50), DELEN(50), PICDIM13
*          1 TNBS(1130,3), NBS(12), CBS3(4,4), ABS3(4,4), BBS3(4,4), CFP02(6,12), CFP03(12,20), PICDIM14
*          2 CFP11(2,6), CFP12(6,12), CFP13(12,20), BEBS3(4,4), GBS4(12,6), PICDIM15
*          3 CBS3(4,4), ALBS3(4,4), BEBS3(4,4), JBS4(4,4), GBS4(12,6), PICDIM16
*          4 GBS5(12,6), GBS6(8,3), GBS7(11,4), GBS8(11,5), EIONK(11), EIONE(11), CORE(7,10), KLK(10,5), EPKL(25), GAUNT(24,25), PICDIM17
*          5 SIGHE(50), ZSC(4200), CSC(4200), KX(620), KTA(620), PICDIM18
*          6 IMA(620), NLSC(620), KY(620), NN(20), TT(20), SPEC(8), PICDIM19
*          7 XN=CORE(2,K), PICDIM19
*          8 L=CORE(3,K), PIC 2
*          N=XMIN1F(XN,10.0), PIC 3
*          DO 100 J=1, NEN, PIC 4
*          E=DELEN(J)/(XN*XN*OMEGAT), PIC 5
*          PHSIG(J)=107.57*OMEGAT**2/(XN*(OMEGAT+DELEN(J))**3)*PGAUNT(N,L,E)*PIC 6
*          1 CORE(6,K), PIC 7
*          100 CONTINUE, PIC 8
*          IGC=CORE(1,K), PIC 9
*          NI=N, PIC 10
*          LI=L, PIC 11
*          ISC=CORE(4,K), PIC 12
*          LC=CORE(5,K), PIC 13
*          FPSQ=CORE(6,K), PIC 14
*          RETURN, PIC 15
*          END

```

```

* FORTRAN
* FUNCTION PGAUNT(N,L,E)
* EVALUATES GAUNT FACTOR FROM KARZAS-LATTER TABLES
* COMMON NOMEGA, DOMEGA, NRHO, ALPHAO, TEMP, K1, K2, IGZERO, PICCOMM1
* 1 NZERO, LZERO, KSZERO, LAZERO, IBETA, EZERO, EKZERO, NS, NP, L12, PICCOMM2
* 2 IS12, ISPEC, JSPEC, ZRES, ZNUCL, NTOTAL, NIC, ZETANU, OMEGAT, PICCOMM3
* 3 XNUI, XMUI, XEPI, IGC, NI, LI, ISC, LC, FPSQ, NEN, NPI, NENY, PICCOM 4
* 4 DENS, EDENS, SLIM, PIEDGE, ALPHA, PHSIG, DELEN, PICCOM 5
* 5 TNBS, NBS, CFP01, CFP02, CFP03, CFP11, CFP12, CFP13, ABS3, CBS3, ALBS3, PICCOM16
* 6 BEBS3, JBS4, GBS4, GABS5, GBS6, GBS7, EIONK, EIONE, CORE, KLK, EPKL, PICCOM17
* 7 GAUNT, SIGHE, IMA, NLSC, KX, NSC, ZSC, CSC, NFUNCT, KTAB, NWFCTS, KY
* DIMENSION DENS(6), EDENS(6), SLIM(6), PIEDGE(6), ALPHA(6), PICDIM 1
* 1 PHSIG(50), DELEN(50), PICDIM 2
* 2 TNBS(1130,3), NBS(12), CBS3(12), CFP01(2,6), CFP02(6,12), CFP03(12,20), PICDIM13
* 3 CFP11(2,6), CFP12(6,12), CFP13(12,20), ABS3(4,4), BBS3(4,4), PICDIM14
* 4 CBS3(4,4), ALBS3(4,4), BEBS3(4,4), JBS4(4,4), GBS4(12,6), PICDIM15
* 5 GABS5(12,6), GBS6(8,3), GBS7(11,4), GBS8(11,5), EIONK(11), PICDIM16
* 6 EIONE(11), CORE(7,10), KLK(10,5), EPKL(25), GAUNT(24,25), PICDIM17
* 7 SIGHE(50), ZSC(4200), CSC(4200), KX(620), KTAB(620), PICDIM18
* 8 IMA(620), NLSC(620), KY(620), NN(20), ZT(20), CI(20), SPEC(8), PICDIM19
* LLL = L + 1
* K = KLK(N,LLL)
* IF(K) 200,200, 5
* 5 IF(E-EPKL(1)) 10, 10, 20
* 10 PGAUNT=GAUNT(K,1)
* 10 RETURN
* 20 DO 50 NX=1,25
* 20 IF(E-EPKL(NX)) 30, 30, 50
* 30 PGAUNT=GAUNT(K,N,-1)+(E-EPKL(NX-1))*(GAUNT(K,NX)-GAUNT(K,NX-1))/1
* 1 (EPKL(NX)-EPKL(NX-1))
* 1 GO TO 100
* 50 CONTINUE
* 60 PGAUNT=GAUNT(K,25)
* 100 RETURN
* 200 WRITE OUTPUT TAPE 6,1000, K1, K2, IGZERO, NZERO, LZERO,
* 1 KSZERO, LAZERO, IBETA, EZERO, N, L, E, CORE

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```
PGAUNT=0.0
RETURN
1000 FORMAT(13H1GAUNT ERROR- 211, 212, 411,1PE20.8, 215,E20.8/(6E20.8))PGAUNTF1
END
PGAUNT15
PGAUNT16
PGAUNT17
```

FORTRAN

* SUBROUTINE PIBS(K)

C EVALUATES BURGESS-SEATON CROSS SECTION FOR KTH-CORE-
 COMMON NOMEGA, OMEGA0, DOMEGA, NRHO, ALPHA0, TEMP, K1, K2, IGZERO, PICCOM1
 1 NZERO, LZERO, KSZERO, LAZERO, IBETA, EZERO, EKZERO, NS, NP, L12, PICCOM2
 2 IS12, ISPEC, ZRES, ZNUCL, NTOTAL, NIC, ZETANU, OMEGAT, PICCOM3
 3 XNU1, XMUI, XEPI, IGC, NI, LI, ISC, LC, FPSQ, NEN, NPI, NENY, PICCOM4
 4 DENS, EDENS, SLIM, PIEDGE, ALPHA, PHSIG, DELEN, PICCOM5
 5 TNBS, NBS, CFP01, CFP02, CFP03, CFP11, CFP12, CFP13, ABS3, CBS3, ALBS3, PICCOM16
 6 BEBS3, JBS4, GBS4, GABS5, GBS5, GBS7, GBS8, EIONK, EIONE, CORE, KLK, EPKL, PICCOM17
 7 GAUNT, SIGHE, IMA, NLSC, KX, NSC, ZSC, CSC, NFUNCT, KTAB, NWFCTS, KY PICCOM18
 DIMENSION DENS(6), EDENS(6), SLIM(6), PIEDGE(6), ALPHA(6), PICDIM1
 1 PHSIG(50), DELEN(50), PICDIM2
 2 TNBS(1130,3), NBS(12), CFP01(2,6), CFP02(6,12), CFP03(12,20), PICDIM13
 3 CFP11(2,6), CFP12(6,12), CFP13(12,20), ABS3(4,4), BB53(4,4), PICDIM14
 4 CBS3(4,4), ALBS3(4,4), BEBS3(4,4), JBS4(4,4), GBS4(12,6), PICDIM15
 5 GABS5(12,6), GBS6(8,3), GBS7(11,4), GBS8(11,5), EIONK(11), PICDIM16
 6 EIONE(11), CORE(7,10), KLK(10,5), EPKL(25), GAUNT(24,25), PICDIM17
 7 SIGHE(50), ZSC(4200), CSC(4200), KX(620), KTAB(620), PICDIM18
 8 IMA(620), NLSC(620), KY(620), NN(20), ZT(20), C1(20), SPEC(8), PICDIM19
 9 XVECT(5), CLEBS(3), AQD(3), PMU(10), EPMU(10), DIF(10), PICDS D8
 CALL BSNORM(K), PICBS 1
 KST=KSZERO, PICBS A1
 LST=LZERO, PICBS A1
 LI=LI, PICBS 2
 DO 900 I=1,3,2, PICBS 3
 SIGMA0=.8559/ZETANU*(XNU1/ZRES)**2, PICBS 4
 NQD=0, PICBS 5
 CLEBS(J)=0.0, PICBS 6
 10 AQD(J)=0.0, PICBS 7
 LEP=LI-2+1, PICBS 8
 11 F(LEP) 900, 12, 12, PICBS 9
 12 IF(INI=4) 20, 14, 14, PICBS A9
 14 IF(KST) 15, 15, 16, PICBS B9
 15 KST=9, PICBS C9

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16 IF(LST) 18, 18, 20
18 LST=9
20 C=2*LI+1
C=MAXOF(LI,LEP)/C*FPSQ
1F(NI-2) 22, 22, 25
22 IF(NZERO-2) 25, 25, 40
25 IF(ISC-1) 50, 30, 50
30 IF(LC) 50, 40, 50
40 NQD=1
CLEBS(2)=C
GO TO 100
50 IF(LEP-2) 55, 40, 40
55 IF(LST -9) 60, 40, 40
60 DO 90 J=1,3
LAP=LST -2+J
1F(XABSF(LAP-LC)-LEP) 65, 65, 90
65 NQD=NQD+1
70 Z=(2*LI+1)*(2*LAP+1)
CLEBS(J)=Z*C*RACAH(LI,LEP,LST
,AQD(J)=PHASE(K1,K2,IGC,LEP,KST
, ,LAP,CORE(7,K))
90 CONTINUE
100 Z=LI+2
1F(XNU1-Z)110, 300, 300
110 IF(LI-1) 400, 120, 300
120 IF(LEP-1) 500, 500, 600
200 SIGMA=SIGMA0*G*G
GAMMA=2.0*GAMMA-1.0
XNU2=XNU1*XNU1
ALFA=ALFA*XNU1
BETA=BETA*XNU2
CHI=CHI+XNU1
210 DO 250 N=1,NEP
DELEN(N)/(13.605*ZRES**2)
Y=CHI+ALFA*EP/(1.0+XNU1*EP)+BETA*EP/(1.0+XNU2*EP)
X=SIGMA/(1.0+XNU2*EP)**GAMMA
C=0.0
PICBS D9
PICBS E9
PICBS 10
PICBS 11
PICBSA11
PICBSB11
PICBS 12
PICBS 13
PICBS 14
PICBS 15
PICBS 16
PICBS 17
PICBS 18
PICBS 19
PICBS 20
PICBS 21
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PICBS 31
PICBS 32
PICBS 33
PICBS 34
PICBS 35
PICBS 36
PICBS 37
PICBS 38
PICBS 39
PICBS 40
PICBS 41

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220 DO 230 J=1,3
225 Z=COSF(3.14159*(Y+AOD(J)))**2
230 C=C+CLEBS(J)*Z
      PHSIG(N)=PHSIG(N)+X*C
250 CONTINUE
      IF(1BETA-9) 900, 260, 260
260 WRITE OUTPUT TAPE 6, 1000, K1, K2, IGZERO, NZERO, LZERO, KSZERO, PICBS 43
      1 LAZERO, IBETA, K, XNUI, ZETANU, SIGMA, ALFA,BETA,CHI,LEP,PICBS 44
      2 L,I
270 DO 280 J=1,3
      LAP=LAZERO-2+J
      WRITE OUTPUT TAPE 6, 1100, LAP, CLEBS(J), AOD(J)
280 CONTINUE
900 CONTINUE
      RETURN
300 LIP = LI + 1
      LEPP = LEP + 1
      CHI=ABS3(LIP ,LEPP )+BBS3(LIP ,LEPP )/XNUI+CBS3(LIP ,LEPP )/
      1 XNUI**2
      ALFA=ALBS3(LIP ,LEPP )
      BETA=BEB3(LIP ,LEPP )
310 NU=XNUI
      J=JBS4(LIP ,LEPP )
      IF(J) 312, 312, 315
312 WRITE OUTPUT TAPE 6, 1200
      GO TO 260
315 IF(NU) 320, 320, 325
320 G=GBS4(1,J)+(XNUI-1.0)*(GBS4(2,J)-GBS4(1,J))
      GAMMA=GABSS(1,J)+(XNUI-1.0)*(GABSS(2,J)-GABSS(1,J))
      GO TO 200
325 IF(NU-12) 340, 330, 330
330 G=GBS4(12,J)
      GAMMA=GABSS(12,J)
      GO TO 200
340 G=GBS4(NU,J)+(XNUI-FLOATF(NU))*(GBS4(NU+1,J)-GBS4(NU,J))

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GAMMA=GABSS5(NU,J)+(XNUI-FLOATF(NU))*(GABSS5(NU+1,J)-GABSS5(NU,J)) PICCBS318
GO TO 200 PICCBS319
400 ALFA=.310 PICCBS400
BETA=0.0 PICCBS401
NU=5.0*(XNUI-.4) PICCBS402
IF(NU) 410, 410, 420 PICCBS403
410 G=GBS6(1,1)+(XNUI-0.6)*(GBS6(2,1)-GBS6(1,1))*5.0 PICCBS407
GAMMA=GBS6(1,2)+(XNUI-0.6)*(GBS6(2,2)-GBS6(1,2))*5.0 PICCBS408
CHI=GBS6(1,3)+(XNUI-0.6)*(GBS6(2,3)-GBS6(1,3))*5.0 PICCBS409
GO TO 200 PICCBS410
420 Y=.2*FLOATF(NU)+.4 PICCBS411
DO 425 J=1,3 PICCBS412
425 XVECT(J)=GBS6(NU,J)+(XNUI-Y)*(GBS6(NU+1,J)-GBS6(NU,J))*5.0 PICCBS413
G=XVECT(1) PICCBS414
GAMMA=XVECT(2) PICCBS415
CHI=XVECT(3) PICCBS416
GO TO 200 PICCBS417
500 ALFA=0.0 PICCBS500
BETA=0.0 PICCBS501
NU=5.0*(XNUI-.8) PICCBS502
IF(NU) 510, 510, 520 PICCBS503
510 SIGMA0=SIGMA0*XNUI*(XNUI+1.0)*ZETANU/(XNUI+2.0) PICCBS504
DO 515 J=1,4 PICCBS505
515 XVECT(J)=GBS7(1,J)+(XNUI-1.0)*(GBS7(2,J)-GBS7(1,J))*5.0 PICCBS507
G=XVECT(1) PICCBS508
GO TO 540 PICCBS509
520 Y=.2*FLOATF(NU)+.8 PICCBS510
DO 525 J=1,4 PICCBS511
525 XVECT(J)=GBS7(NU,J)+(XNUI-Y)*(GBS7(NU+1,J)-GBS7(NU,J))*5.0 PICCBS512
IF(XNUI-1.6) 530, 530, 535 PICCBS513
530 G=SQRTF(XNUI-1.0)*XVECT(1) PICCBS514
GO TO 540 PICCBS515
535 G=XVECT(2) PICCBS516
540 GAMMA=XVECT(3) PICCBS517
CHI=XVECT(4) PICCBS518
GO TO 200

```

```

600  ALFA=.362
     NU=.5* (XNUI-.8)
     IF (NU) 610, 610, 620
610  SIGMA0=SIGMA0*XNUI*(XNUI+1.)*ZETANU/(XNUI+2.)
     DO 615 J=1,5
615  XVECT(J)=GBS8(1,J)+(XNUI-1.0)*(GBS8(2,J)-GBS8(1,J))*5.0
     G=XVECT(1)
     GO TO 640
620  Y=.2*FLOATF(NU)+.8
     DO 625 J=1,5
625  XVECT(J)=GBS8(NU,J)+(XNUI-Y)*(GBS8(NU+1,J)-GBS8(NU,J))*5.0
     IF (XNUI-1.6) 630, 635
630  G=SQRTF(XNUI-1.0)*XVECT(1)
     GO TO 640
635  G=XVECT(2)
640  GAMMA=XVECT(3)
     CHI=XVECT(4)
     BETA=XVECT(5)
     GO TO 200
200  FORMAT(28H1BURGESS-SEATON CALCULATION-/5X2HID,7X1HK,9X2HNU,11X4HZEPICBS
     1TA,10X5HSIGMA,10X5H GAMMA,10X5HALPHA,11X4HBETA,12X3HCHI/12,11,212, PICBS
     2 411,14,1P7E15.4//1H ,6X8HL(PRIME),6X5HCLEBS,7X27HEXTRAPOLATED QUAPICBS
     3NTUM DEFECT,10X4HLEP=,I4,10X3HLI=,I4)
     1100 FORMAT(115,1PE15.4,1PE30.4)
     1200 FORMAT(11H1BS300-, J=0)
     1050 FORMAT(20H0 ELECTRON ENERGY,7X,13HCROSS SECTION//(1P2E20.8))
     END

```

```

*          FORTRAN          0
*          SUBROUTINE BSNORM (K)
C          EVALUATE NORMALIZATION OF BOUND STATE RADIAL WAVE FUNCTION
COMMON NOMEGA, OMEGA0, DOMEGA, NRHO, ALPHA0, TEMP, K1, K2, IGZERO, PICCOMM1
1  NZERO,LZERO, KSZERO, LAZERO, IBETA, EZERO, EKZERO, NS, NP, L12, PICCOMM2
2  IS12, ISPEC, JSPEC, ZRES, ZNUCL, NTOTAL, NIC, ZETANU, OMEGAT, PICCOMM3
3  XNUI,XMUI,XEPI,IGC,NI,LI,ISC,LC,FPSQ, NEN, NPI, NENY, PICCOM 4
4  DENS, EDENS,SLIM, PIEDGE, ALPHA, PHSIG, DELEN, PICCOM 5
5  TNBS,NBS,CFP01,CFP02,CFP03,CFP11,CFP12,CFP13,ABS3,BBS3,CBS3,ALBS3,PICCOM16
6  BEBS3,JBS4,GBS4,GABSS5,GBS6,GBS7,GBS8,EIONK,EIONE, CORE, KLK,EPKL, PICCOM17
7  GAUNT,SIGHE,IMA,NLSC,KX,NSC,ZSC,CSC,NFUNCT,KTAB,NWFCTS,KY
DIMENSION DENS(6), EDENS(6), SLIM(6), PIEDGE(6), ALPHA(6),
1  PHSIG(50), DELEN(50),
2  TNBS(1130,3), NBS(12), CFP01(2,6), CFP02(6,12), CFP03(12,20),
3  CFP11(2,6), CFP12(6,12), CFP13(12,20), ABS3(4,4), BBS3(4,4),
4  CBS3(4,4), ALBS3(4,4), BEBS3(4,4), JBS4(4,4), GBS4(12,6),
5  GABSS5(12,6), GBS6(8,3), GBS7(11,4), GBS8(11,5), EIONK(11),
6  EIONE(11), CORE(7,10), KLK(10,5), EPKL(25), GAUNT(24,25),
7  SIGHE(50),
8  IMA(620), NLSC(620), KY(620), NN(20), ZT(20), CI(20), SPEC(8)
1  IGC=CORE(1,K)
NI=CORE(2,K)
LI=CORE(3,K)
1  ISC=CORE(4,K)
LC=CORE(5,K)
FPSQ=CORE(6,K)
10 XNUI=ZRES*SQRRTF(109737.3/(CORE(7,K)-EKZERO))
XMUI=CORE(2,K)-XNU1
XEPI=-1.0/XNU1**2
20 IST=KSZERO
LAT=LAZERO
30 IF(NI=4) 50, 35, 35
35 IF(IST) 40, 37, 40
37 IST=9
40 IF(LAT) 50, 45, 50
45 LAT=9
BSNORM 0
BSNORMC1
BSNORM 1
BSNORM 2
BSNORM 3
BSNORM 4
BSNORM 5
BSNORM 6
BSNORM 7
BSNORM 8
BSNORM 9
BSNORM10
BSNORM11
BSNORM12
BSNORM13
BSNORM14
BSNORM15
BSNORM16

```

```

50 IF(NI-2) 100, 100, 200
100 IF(NZERO-2) 105, 105, 150
105 IF(LI) 120, 110, 120
110 IF(LLZERO) 125, 115, 125
115 ZETANU=ZETA(K1,K2,IGC,NI+1,LI,IST,LAT,CORE(7,K))
      RETURN
120 IF(XNUI-1.) 125, 125, 128
125 ZETANU=1.0
      RETURN
129 IF(XNUI-1.2) 130, 130, 132
130 X=1.0
      GO TO 134
132 X=ZETA(K1,K2,IGC,3,LI,IST,LAT,CORE(7,K))
134 ZETANU=(XNUI-1.)*(XNUI+2.)/(XNUI*(XNUI+1.))
      IF(X-1.) 135, 138, 135
135 ZETANU=.5*(ZETANU+X)
138 RETURN
150 IF(LI) 155, 125, 155
155 IF(XNUI-1.) 125, 125, 160
160 ZETANU=(XNUI-1.)*(XNUI+2.)/(XNUI*(XNUI+1.))
      RETURN
200 IF(LI-NI+1) 220, 210, 220
210 ZETANU=ZETA(K1,K2,IGC, NI+1,LI,IST, LAT, CORE(7,K))
      RETURN
220 IF(NI-3) 250, 230, 250
230 IF(LI) 240, 210, 240
240 IGP=IGAMMA(1SPEC,NS,9,9)
      GO TO 260
250 IGP=IGC
260 X=ZETA(K1,K2,IGP,NI-1,LI, IST, LAT, CORE(7,K))
      Y=ZETA(K1,K2,IGC,NI+1,LI, IST, LAT, CORE(7,K))
      IF(X-1.) 270, 285, 270
270 IF(Y-1.) 280, 290, 280
280 ZETANU=.5*(X+Y)
      RETURN
285 ZETANU=Y

```


* FORTRAN

```

FUNCTION QDE (IX1, IX2, IGAM, N, L, ISBAR, LTOT, ELIM)      QDEF 0
COMMON NOMEA, OMEGA, DOMEA, NRHO, ALPHA0, TEMP, K1, K2, IGZERO, PICCOM1
1  NZERO, LZERO, KSZERO, LAZERO, IBETA, EZERO, EKZERO, NS, NP, L12, PICCOM2
2  IS12, ISPEC, JSPEC, ZRES, ZNUCL, NTOTAL, NIC, ZETANU, OMEGAT, PICCOM3
3  XNUI, XMUI, XEPI, IGC, NI, LI, ISC, LC, FPSQ, NEN, NPI, NENGY, PICCOM4
4  DENS, EDENS, SLIM, PIEDGE, ALPHA, PHSIG, DELEN, PICCOM5
5  TNBS, NBS, CFP01, CFP02, CFP03, CFP11, CFP12, CFP13, ABS3, BBS3, CBS3, PICCOM6
6  BEBS3, JBS4, GBS4, GABSS, GBS6, GBS7, GBS8, EIONK, EIONE, CORE, KLK, EPKL, PICCOM7
7  GAUNT, SIGHE, IMA, NLSC, KX, NSC, ZSC, CSC, NFUNC, KTAB, NWFC, KY, PICCOM8
DIMENSION DENS(6), EDENS(6), SLIM(6), PIEDGE(6), ALPHA(6), PICCOM9
PCDIM1
```

- 1 PHSIG(50), DELEN(50),
- 2 TNBS(1130,3), NBS(12), CFP01(2,6), CFP02(6,12), CFP03(12,20), PICDIM2
- 3 CFP11(2,6), CFP12(6,12), CFP13(12,20), ABS3(4,4), BBS3(4,4), PICDIM3
- 4 CBS3(4,4), ALBS3(4,4), BEBS3(4,4), JBS4(4,4), GBS4(12,6), PICDIM4
- 5 GABS5(12,6), GBS6(8,3), GBS7(11,4), GBS8(11,5), EIONK(11), PICDIM5
- 6 EIONE(11), CORE(7,10), KLK(10,5), EPKL(25), GAUNT(24,25), PICDIM6
- 7 SIGHE(50), ZSC(4200), CSC(4200), KX(620), KTAB(620), PICDIM7
- 8 IMA(620), NLSC(620), KY(620), NN(20), ZT(20), CI(20), SPEC(8), PICDIM8
- X=ESPEC(IX1, IX2, IGAM, N, L, ISBAR, LTOT) PICDIM9
- QDEF 1

- 1 IF(X) 20, 50, 50
- 20 QDE =-1.0
- 20 RETURN
- 50 QDE =ZRES*SQRTF(109737.3/(ELIM-X))
- 50 RETURN
- END

* FORTRAN FUNCTION RACAH(IAP,IBP,ICP,IEP,LC)
 C COMPUTES RACAH COEFFICIENT (BURGESS-SEATON TABLE 1•)
 IF(IAP-IBP) 150, 150, 100

```

100  IA=IBP          PIBSR 0
     IB=IBP          PIBSR 1
     IC=IEP          PIBSR 10
     IE=IEP          PIBSR 20
     GO TO 200       PIBSR 30
150  IA=IAP          PIBSR 40
     IB=IBP          PIBSR 50
     IC=IEP          PIBSR 60
     IE=IEP          PIBSR 61
     GO TO 200       PIBSR 62
200  IF(IC-IE) 300, 400, 500
     XN=(LC+IC+IA+3)*(LC+IC+IA+2)*(IC+IA+2-LC)*(IC+IA+1-LC)
     D=4*(2*IC+3)*(IC+1)*(2*IC+1)*(2*IA+3)*(IA+1)*(2*IA+1)
     GO TO 600       PIBSR 7
300  XN=(LC+IC+IA+2)*(IC+IA+1-LC)*(LC-IC+IA+1)*(LC+IC-IA)
     D=4*IC*(2*IC+1)*(IC+1)*(2*IA+1)*(IA+1)*(2*IA+3)
     GO TO 600       PIBSR 8
400  XN=(LC+IC-IA)*(LC+IC-IA-1)*(LC-IC+IA+2)*(LC-IC+IA+1)
     D=4*(2*IC+1)*(2*IC-1)*(IA+1)*IC*(IA+1)*(2*IA+3)
     GO TO 600       PIBSR 9
500  XN=(LC+IC-IA)*(LC+IC-IA-1)*(LC-IC+IA+2)*(LC-IC+IA+1)
     D=4*(2*IC+1)*(2*IC-1)*(IA+1)*(2*IA+1)*(2*IA+3)
600  RACAH=XN/D      PIBSR 10
     RETURN          PIBSR 11
     END             PIBSR 12
                                PIBSR 13
                                PIBSR 14
                                PIBSR 15
                                PIBSR 16
                                PIBSR 17
                                PIBSR 18
  
```

FORTRAN

```
0
PICMU 0
PICMU C1
PICCOMM1
PICCOMM2
PICCOMM3
PICCOM 4
PICCOM 5
PICDIM 2
PICDIM 13
PICDIM 14
PICDIM 15
PICDIM 16
PICDIM 17
PICDIM 18
PICDIM 1
PICDIM 2
PICMU 1
PICMU 2
PICMU 3
PICMU 4
PICMU 5
PICMU 6
PICMU 7
PICMU 8
PICMU 9
PICMU 10
PICMU 11
PICMU 12
PICMU 13
PICMU 14
PICMU 15
0
FUNCTION PHASE(IX1):=(2,IGAM,L,IS,LA,ELIM)
EVALUATE ZERO ENERGY QUANTUM DEFECT (PHASE SHIFT)
COMMON NOMEKA, OMEGA0, DOMEKA, NRHO, ALPHAO, TEMP, K1, K2, IGZERO, PICCOMM1
NZERO, LZERO, KSZERO, LAZERO, IBETA, EZERO, EKZERO, NS, NP, L12, PICCOMM2
1 IS12, ISPEC, ZRES, ZNUCL, NTOTAL, NIC, ZETANU, OMEGAT, PICCOMM3
2 3XNU1, XNU1, XEP1, IGC, NI, LI, ISC, LC, FPSQ, NEN, NPI, NENY,
3XNU1, XNU1, XEP1, IGC, NI, LI, ISC, LC, FPSQ, NEN, NPI, NENY,
4DENS, EDENS, SLIM, PIEDGE, ALPHA, FHSIG, DELEN,
5TNBS, NSS, CFP01, CFP02, CFP03, CFP11, CFP12, CFP13, ABS3, BBS3, CBS3, ALBS3, PICCOM16
6BBS3, JBS4, GBS5, GBS6, GBS7, GBS8, EIONK, EIONE, CORE, KLK, EPKL, PICCOM17
7GAUNT, SIGHE, IMA, NLSC, KX, NSC, ZSC, CSC, NFUNCNT, KTAB, NWFCTS, KY
8DIMENSION DENS(6), EDENS(6), SLIM(6), PIEDGE(6), ALPHA(6),
9PHS, IG(50), DELEN(50),
10TNBS(1130,3), NBS(12), CFP01(2,6), CFP02(6,12), CFP03(12,20),
11CFP11(2,6), CFP12(6,12), CFP13(12,20), ABS3(4,4), BBS3(4,4),
12CBS3(4,4), ALBS3(4,4), BEBS3(4,4), JBS4(4,4), GBS4(12,6),
13GBS5(12,6), GBS6(8,3), GBS7(11,4), GBS8(11,5), EIONK(11),
14EIONE(11), CORE(7,10), KLK(10,5), EPKL(25), GAUNT(24,25),
15SIGHE(50),
16IMA(620), NLSC(620), KY(620), NN(20), ZT(20), CI(20), SPEC(8),
17PMU(10), EPMU(10), DIF(10),
18ISP=IS
19LP=LA
20NQ=0
21DC 10 J=1,10
22PMU(J)=0.0
23EPMU(J)=0.0
24DIF(J)=0.0
25DC 30 NX=3,12
26X=QDE (IX1,IX2,IGAM, NX, L, ISP, LP, ELIM)
27IF (X)100,100, 20
28NQ=NQ+1
29PMU(NQ)=FLOATF(NX)-X
30EPMU(NQ)=-1.0/X**2
31CONTINUE
32NPX=NQ-1
```

```

DO 40 J=1,NPX
40 DIF(J)=(PMU(J+1)-PMU(J))/(EPMU(J+1)-EPMU(J))
IF(NQ-3) 50, 50, 60
50 PHASE=PMU(NQ)-EPMU(NQ)*DIF(NQ-1)
GO TO 200
60 NPX=NQ-2
DO 85 J=2,NPX
IF(DIF(J)) 65, 80, 80
65 IF(DIF(J+1)) 85, 85, 70
70 X=NQ-1
Y=0.0
DO 75 J=2,NQ
75 Y=Y+PMU(J)
PHASE=Y/X
GO TO 200
80 IF(DIF(J+1)) 70, 85, 85
85 CONTINUE
GO TO 50
100 IF(NQ-2) 110, 35, 35
110 IF(ISP-9) 120, 125, 125
120 ISP=9
GO TO 5
125 IF(LP-9) 130, 140, 140
130 LP=9
GO TO 5
140 IF(NQ) 150, 150, 145
145 PHASE=PMU(NQ)
GO TO 200
150 PHASE=0.0
200 RETURN
END

```

```

* * * * * FORTRAN SUBROUTINE PIHE(K)
* * * * * EVALUATES HIGH-ENERGY ACCELERATION BORN APPROXIMATION
* * * * * PHOTOIONIZATION CROSS SECTION FOR KTH-CORE-
* * * * * COMMON NOMEGA, OMEGA0, DOMEGA, NRHO, ALPHA0, TEMP, K1, K2, IGZERO, PICCOMM1
* * * * 1 NZERO, LZERO, KSZERO, LAZERO, IBETA, EZERO, EKZERO, NS, NP, L12, PICCOMM2
* * * * 2 IS12, ISPEC, JSPEC, ZRES, ZNUCL, NTOTAL, NIC, ZETANU, OMEGAT, PICCOMM3
* * * * 3 XNU1, XMUI, XEPI, IGC, NI, LI, ISC, LC, FPSQ, NEN, NPI, NENGY, PICCOMM4
* * * * 4 DENS, EDENS, SLIM, PIEDGE, ALPHA, PHSIG, DELEN, PICCOMM5
* * * * 5 TNBS, NBS, CFP01, CFP02, CFP03, CFP11, CFP12, CFP13, ABS3, CBS3, ALBS3, PICCOMM16
* * * * 6 BEBS3, JBS4, GBS4, GABSS5, GBS5, GBS6, GBS7, GBS8, EIONK, EIONE, CORE, KLK, EPKL, PICCOMM17
* * * * 7 GAUNT, SIGHE, IMA, NLS, KX, NSC, ZSC, CSC, NFUNCT, KTAB, NWFCTS, KY, PICCOMM18
* * * * DIMENSION DENS(6), EDENS(6), SLIM(6), PIEDGE(6), ALPHA(6), PICDIM1
* * * * PHSIG(50), DELEN(50), PICDIM2
* * * * 2 TNBS(1130,3), NBS(12), CFP01(2,6), CFP02(6,12), CFP03(12,20), PICDIM13
* * * * 3 CFP11(2,6), CFP12(6,12), CFP13(12,20), ABS3(4,4), BBS3(4,4), PICDIM14
* * * * 4 CBS3(4,4), ALBS3(4,4), BEBS3(4,4), JBS4(4,4), GBS4(12,6), PICDIM15
* * * * 5 GABSS5(12,6), GBS6(8,3), GBS7(11,4), GBS8(11,5), EIONK(11), PICDIM16
* * * * 6 EIONE(11), CORE(7,10), KLK(10,5), EPKL(25), GAUNT(24,25), PICDIM17
* * * * 7 SIGHE(50), ZSC(4200), CSC(4200), KX(620), KTAB(620), PICDIM18
* * * * 8 IMA(620), NLS(620), KY(620), NN(20), ZT(20), CI(20), SPEC(8), PICDIM19
* * * * 1 IGC=CORE(1,K)
* * * * 2 NI=CORE(2,K)
* * * * 3 LI=CORE(3,K)
* * * * 4 ISC=CORE(4,K)
* * * * 5 LC=CORE(5,K)
* * * * FPSQ=CORE(6,K)
* * * * 10 CALL SLACIK2, NS, NP, NZERO, LZERO, NI, LI, NN, ZT, CI, NBASIS
* * * * DO 15 J=1,NBASIS
* * * * X=FACTO(2*NN(J));
* * * * CI(J)=2*Z1(J)*NN(J)*SQRTF(2.0*ZT(J),X)*CI(J)
* * * * 15 NN(J)=NN(J)-1
* * * * DO 500 I=1,3,2
* * * * 20 LEP=LI-2+1
* * * * IF(LEP) 500, 30, 30
* * * * 30 C=MAXOF(IL,LEP)/FLOATF(2*LI+1)

```

```

SIGMA0=1.712*FPSQ*C*ZNUCL**2
DO 400 N=2,NEN
40 EK=SQRTF(DELLEN(N)/13.605)
WAVE=(DELLEN(N)+OMEGAT)/27.21
X=0.0
DO 200 J=1,NBASIS
X=X+C1(J)/EK**NN(J)*BESS(ZT(J)/EK,NN(J), LEP,4.0*ZRES/EK)
200 CONTINUE
SIGHE(N)=SIGHE(N)+SIGMA0/WAVE**3*X**2/EK
400 CONTINUE
500 CONTINUE
IF(IBETA-9) 900, 600, 600
600 WRITE OUTPUT 6, 1000, K1, K2, IZERO, NZERO, LZERO, KSZERO,
1 LAZERO, IBETA, K, (NN(J),ZT(J), CI(J), J=1,NBASIS)
900 RETURN
1000 FORMAT(31H8ACCELERATION BORN CALCULATION-/5X2HID,7X1HK/I2,I1,212,
1 4I1,I4//15H BOUND STATE-,9X1HN,12X4HZETA,13X11HCOEFFICIENT/
2 (I25,1P2E20.4))
END

```

* FORTTRAN

SUBROUTINE SLAC(IX2,NSSLAC,NPSLAC,NSLAC,NO,LO,NN,ZT,CI,
1NBASIS)

```

COMMON NOMEA, OMEAO, DOMEA, NRHO, ALPHAO, TEMP, K1, K2, IGZERO, PICCOMM1
1 NZERO, LZERO, KSZERO, LAZERO, IBETA, EZERO, EKZERO, NS, NP, L12, PICCOMM2
2 IS12, ISPEC, JSPEC, ZRES, ZNUCL, NTOTAL, NIC, ZETANU, OMEGAT, PICCOMM3
3 XNUI, XMUI, XEPI, IGC, NI, LI, ISC, LC, FPSQ, NEN, NPI, NENY, PICCOMM4
4 DENS, EDENS, SLIM, PIEDGE, ALPHA, PHSIG, DELEN, PICCOMM5
5 TNBS, NBS, CFP01, CFP02, CFP03, CFP11, CFP12, CFP13, ABS3, CBS3, ALBS3, PICCOMM6
6 BEBS3, JBS4, GBS4, GABS5, GBS5, GBS6, GBS7, GBS8, EIONK, EIONE, CORE, KLK, EPKL, PICCOMM7
7 GAUNT, SIGHE, IMA, NLSC, KX, NSC, ZSC, CSC, NFUNCT, KTAB, NWFCTS, KY, PICCOMM8
DIMENSION DENS(6), EDENS(6), SLIM(6), PIEDGE(6), ALPHA(6), PICDIM1
1 PHSIG(50), DELEN(50), PICDIM2
2 TNBS(1130,3), NBS(12), CBS3(4,4), ABS3(4,4), CBS4(4,4), ABS4(4,4), PICDIM3
3 CFP1(2,6), CFP12(6,12), CFP13(12,20), ABS3(12,20), CBS3(12,20), PICDIM4
4 CBS3(4,4), ALBS3(4,4), BEBS3(4,4), JBS4(4,4), GBS4(12,6), PICDIM5
5 GABS5(12,6), GBS6(8,3), GBS7(11,4), GBS8(11,5), EIONK(11), PICDIM6
6 EIONE(11), CORE(7,10), KLK(10,5), EPKL(25), GAUNT(24,25), PICDIM7
7 SIGHE(50), ZSC(4200), CSC(4200), KX(620), KTAB(620), PICDIM8
8 IMA(620), NLSC(620), KY(620), NN(20), ZT(20), CI(20), SPEC(8), PICDIM9
IA=IX2*10000
IB=NSSLAC*1000
IC=NPSLAC*100
IFUNCT=IA+IB+IC
IF(NSLAC-2) 3, 3, 2
2 ID=10*XMINOF(NSLAC,8)
IFUNCT=IFUNCT +ID+XMINOF(LSLAC,3)
3 KA=NO*10
NOLO=KA+LO
DO 5 I=1,NWFCTS
IF(IFUNCT-KTAB(1)) 5,20,5
5 CONTINUE
WRITE OUTPUT TAPE 6,1000,IX2,NSSLAC,NPSLAC,NSLAC,NO,LO
GO TO 200
20 K=KX(1)
LK=K+9

```

```
DO 100 J=K,LK
IF(NLSC (J)-NOL0)100,40,100
100 CONTINUE
      WRITE OUTPUT TAPE 6,1100,IX2,NSSLAC,NPSLAC,NSLAC,LSLAC,NO,LO
      GO TO 200
40  NBASIS=IMA(J)
      LIMIT=KY(J)+NBASIS-1
      KK=1
      MN=KY(J)
      DO 150 L=MN,LIMIT
      CALL SUBR2(ZSC(L),ZT(KK),NN(KK))
      CI(KK)=CSC(L)
      KK=KK+1
150  CONTINUE
      RETURN
200  DO 210 J=1,20
210  CI(J)=0.0
      RETURN
1000 FORMAT(30HOSLATER FUNCTION MISSING-KTAB-,7I10)
1100 FORMAT(30HOSLATER FUNCTION MISSING-NLSC-,7I10)
      END
```

```

* FAP COUNT 50
  ENTRY
  SUBR1 SUBR1
    CLA# 1,4
    STO# 3,4
    CAL MASK
    ANS# 3,4
    CAL# 2,4
    ARS 18
    ORS# 3,4
    TRA 4,4
    SUBR2 CAL# 1,4
      ANA MASK
      SLW# 2,4
      CAL# 1,4
      ANA MASK1
      ALS 18
      SLW# 3,4
      TRA 4,4
      MASK OCT 77777777740
      MASK1 OCT 00000000037
      END

```

```
* FORTRAN
FUNCTION FACTO(K)
C COMPUTES K FACTORIAL
FACTO=1.0
IF(K-1) 200, 200, 50
50 DO 100 I=2,K
100 FACTO=FACTO*FLOATF(I)
200 RETURN
END
PIHEF 0
PIHEF 1
PIHEF 2
PIHEF 2
PIHEF 3
PIHEF 4
PIHEF 5
PIHEF 6
```

* FORTRAN

```

FUNCTION BESS(A,J,K,XX)
  COMPUTE INTEGRAL-BESSEL (ORDER=K, EXP.=A, POWER=J)
  COMMON NOMEA, OMEGA, DOMEGA, NRHO, ALPHAO, TEMP, K1, K2, IGZERO, PICCOMM1
  1 NZERO, LZERO, KSZERO, LAZERO, IBETA, EZERO, EKZERO, NS, NP, L12, PICCOMM2
  2 IS12, ISPEC, JSPEC, ZRES, ZNUCL, NTOTAL, NIC, ZETANU, OMEGAT, PICCOMM3
  3 XNUI, XMUI, XEPI, IGC, NI, LI, ISC, LCL, FPSQ, NEN, NPI, NENY,
  4 DENS, EDENS, SLIM, PIEDGE, ALPHA, PHSIG, DELEN, PICCOM 4
  5 STNBS, NBS, CFP01, CFP02, CFP03, CFP11, CFP12, CFP13, ABS3, CBS3, ALBS3, PICCOM16
  6 BEBS3, JBS4, GBS4, GABS5, GBS6, GBS7, GBS8, EIONK, EIONE, CORE, KLK, EPKL, PICCOM17
  7 GAUNT, SIGHE, IMA, NLSC, KX, NSC, ZSC, CSC, NFUNCT, KTAB, NWFCCTS, KY
  DIMENSION DENS(6), EDENS(6), SLIM(6), PIEDGE(6), ALPHA(6),
  1 PHSIG(50), DELEN(50), PICDIM 1
  2 TNBS(1130,3), NBS(12), CFP01(2,6), CFP02(6,12), CFP03(12,20), PICDIM13
  3 CFP11(2,6), CFP12(6,12), CFP13(12,20), ABS3(4,4), BBS3(4,4), PICDIM14
  4 CBS3(4,4), ALBS3(4,4), BEBS3(4,4), JBS4(4,4), GBS4(12,6), PICDIM15
  5 GABS5(12,6), GBS6(8,3), GBS7(11,4), GBS8(11,5), EIONK(11), PICDIM16
  6 EIONE(11), CORE(7,10), KLK(10,5), EPKL(25), GAUNT(24,25), PICDIM17
  7 SIGHE(50),
  8 IMA(620), NLSC(620), KY(620), NN(20), ZT(20), CI(20), SPEC(8), PICDIM18
  9 XVECT(100),
  FBESSF(A,J)=FACTO(J-1)/((A*A+1)**(FLOATF(J)/2.0))
  1 *SINF(FLOATF(J)*ATANF(1.0/A))
  IF(J) 100, 200, 300
  100 WRITE OUTPUT TAPE 6, 1000
  GO TO 410
  200 BESS=BESSO(A,K)
  RETURN
  300 IF(K) 400, 450, 500
  400 WRITE OUTPUT TAPE 6, 1001
  410 BESS=0.0
  RETURN
  450 IF(J-1) 460, 480, 460
  460 BESS=FBESSF(A,J)
  RETURN
  480 BESS=1.0/(1.0+A*A)*EXPF(-XK)
  *ATANF(1.0/A))

```

```
RETURN
500  JP=J+1
505  DO 510  I=2,JP
510  XVECT(I)=FBESSF(A,I-1)
515  DO 610  I=1,K
520  IF(I-3) 530,530, 550
530  XVECT(I)=BESSO(A,I-1)
550  Y=0.0
      DO 600  L=1,JP
560  C=(L+I-2)
      C=C*Y
570  Y=XVECT(L)
600  XVECT(L)=-A*XVECT(L)+C
610  CONTINUE
630  BESS=XVECT(J+1)
      RETURN
1000 FORMAT (20H1J NEGATIVE IN BESS-)
1001 FORMAT (20H1K NEGATIVE IN BESS-)
      END
      PIHEBA14
      PIHEB 15
      PIHEB 15
      PIHEB 16
      PIHEB 17
      PIHEB 17
      PIHEB 18
      PIHEB 19
      PIHEB 20
      PIHEB 21
      PIHEB 22
      PIHEB 23
      PIHEB 24
      PIHEB 25
      PIHEBA25
      PIHEB 26
      PIHEB 27
      PIHEB000
      PIHEB001
      PIHEB
```

```

*      FORTRAN FUNCTION BESSO(A,K)
C      COMPUTES INTEGRAL-BESSEL FOR BETA=0.0.
      IF(K-3)100,200,300
      100  IF(K-1)110,120,130
      110  BESSO=ATANF(1.0/A)
      GO TO 150
      120 BESSO=1.0-A*ATANF(1./A)
      GO TO 150
      130 BESSO=-1.5*A+(1.5*A*A+.5)*ATANF(1./A)
      150 RETURN
      200 BESSO=2.5*A*A+2.0/3.0-(2.5*A*A+1.5)*A*ATANF(1./A)
      RETURN
      300 WRITE OUTPUT TAPE 6,1000
      BESSO=0.0
      RETURN
      1000 FORMAT(27H1K GREATER THAN 3 IN BESSO--)
      END
      PIHEBO 0
      PIHEBO 1
      PIHEBO 2
      PIHEBO 3
      PIHEBO 4
      PIHEBO 5
      PIHEBO 6
      PIHEBO 7
      PIHEBO 8
      PIHEBO 9
      PIHEBO10
      PIHEBO11
      PIHEBO12
      PIHEBO13
      PIHEBO14
      PIHEBO15
      PIHEBO16

```

```

*   FORTRAN SUBROUTINE PIACC
*   COMBINE BURGESS-SEATON AND HIGH-ENERGY CROSS SECTIONS-
*   COMMON NOMEGA, OMEGA0, DOMEGA, NRHO, ALPHA0, TEMP, K1, K2, IGZERO, PICCOMM1
1  NZERO, LZERO, KSZERO, LAZERO, IBETA, EZERO, EKZERO, NS, NP, L12, PICCOMM2
2  IS12, ISPEC, JSPEC, ZRES, ZNUCL, NTOTAL, NIC, ZETANU, OMEGAT, PICCOMM3
3  XNU1, XMUI, XEPI, IGC, NI, LI, ISC, LC, FPSQ, NEN, NPI, NENY, PICCOM 4
4  DENS, EDENS, SLIM, PIEDGE, ALPHA, PHSIG, DELEN, PICCOM 5
5  TNBS, NBS, CFP01, CFP02, CFP03, CFP12, CFP13, ABS3, BBS3, CBS3, ALBS3, PICCOM16
6  BEBS3, JBS4, GBS4, GABS5, GBS6, GBS7, GBS8, EIONK, EIONE, CORE, KLK, EPKL, PICCOM17
7  GAUNT, SIGHE, IMA, NLSC, KX, NSC, ZSC, CSC, NFUNC, KTAB, NWFCTS, KY
8  DIMENSION DENS(6), EDENS(6), SLIM(6), PIEDGE(6), ALPHA(6), PICDIM 1
1  PHSIG(50), DELEN(50), PICDIM 2
2  TNBS(1130,3), NBS(12), CFP01(2,6), CFP02(6,12), CFP03(12,20), PICDIM13
3  CFP11(2,6), CFP12(6,12), CFP13(12,20), ABS3(4,4), BBS3(4,4), PICDIM14
4  CBS3(4,4), ALBS3(4,4), BEBS3(4,4), JBS4(4,4), GBS4(12,6), PICDIM15
5  GABS5(12,6), GBS6(8,3), GBS7(11,4), GBS8(11,5), EIONK(11), PICDIM16
6  EIONE(11), CORE(7,10), KLK(10,5), EPKL(25), GAUNT(24,25), PICDIM17
7  SIGHE(50), ZSC(4200), CSC(4200), KX(620), KTAB(620), PICDIM18
8  IMA(620), NLSC(620), KY(620), NN(20), ZT(20), CI(20), SPEC(8), PICDIM19

DO 10 N=1,5
  SIGHE(N), SIGHE(6)
10 CONTINUE
DO 100 M=1,NEN
  ALFE=(-0.05095)*DELEN(M)/(ZRES*ZRES)
  PHSIG(M)=PHSIG(M)* EXPF(ALFE) + SIGHE(M)*(1.0-EXPF(ALFE))
100 CONTINUE
  RETURN
END

```

```

*          FORTRAN
*          SUBROUTINE PTALLY(IC)
C          TALLY PHOTOIONIZATION TRANSITION IN ATLAS-
COMMON NOMEGA, OMEGA0, NRHO, ALPHA0, TEMP, K1, K2, IGZERO, PICCOMM1
1  NZERO, LZERO, KSZERO, LAZERO, IBETA, EZERO, EKZERO, NS, NP, L12, PICCOMM2
2  IS12, ISPEC, JSPEC, ZRES, ZNUCL, NTOTAL, NIC, ZETANU, OMEGAT, PICCOMM3
3  XNUI, XMUI, XEPI, IGC, NI, LI, ISC, LC, FPSQ, NEN, NPI, NENGY, PICCOM 4
4  DENS, EDENS, SLIM, PIEDGE, ALPHA, PHSIG, DELEN, PICCOM 5
5  TNBS, NBS, CFP01, CFP02, CFP03, CFP11, CFP12, CFP13, ABS3, CBS3, ALBS3, PICCOM16
6  BEBS3, JBS4, GBS4, GABS5, GBS6, GBS7, EIONK, EIONE, CORE, KLK, EPKL, PICCOM17
7  GAUNT, SIGHE, IMA, NLSC, KX, NSC, ZSC, CSC, NFUNCTION, KTAB, NWFCCTS, KY
DIMENSION DENS(6), EDENS(6), S'IM(6), PIEDGE(6), ALPHA(6), PICDIM 1
1  PHSIG(50), DELEN(50), PICDIM 2
2  TNBS(1130, 3), NBS(12), CFP01(2, 6), CFP02(6, 12), CFP03(12, 20), PICDIM13
3  CFP11(2, 6), CFP12(6, 12), CFP13(12, 20), ABS3(4, 4), BBS3(4, 4), PICDIM14
4  CBS3(4, 4), ALBS3(4, 4), BEBS3(4, 4), JBS4(4, 4), GBS4(12, 6), PICDIM15
5  GABS5(12, 6), GBS6(8, 3), GBS7(11, 4), GBS8(11, 5), EIONK(11), PICDIM16
6  EIONE(11), CORE(7, 10), KLK(10, 5), EPKL(25), GAUNT(24, 25), PICDIM17
7  SIGHE(50), ZSC(4200), CSC(4200), KX(620), KTAB(620), PICDIM18
8  IMA(620), NLSC(620), KY(620), NN(20), ZT(20), CI(20), SPEC(8), PICDIM19
9  IF(IBETA-9) 20, 10, 10, PTALLY10
10  WRITE OUTPUT TAPE 6, 15CO, K1, K2, IGZERO, NZERO, LZERO, KSZERO, PTALLY20
1  LAZERO, IBETA, NS, NP, EZERO, (ALPHA(J), J=1, PTALLY30
2  6), IGC, NI, LI, ISC, LC, FPSQ, CORE(7, IC), OMEGAT, (DELEN(1), PTALLY40
3  PHSIG(1), SIGHE(1), I=1, NEN) PTALLY41
20  WRITE TAPE 15, K1, K2, IGZERO, NZERO, LZERO, LAZERO, PTALLY50
1  IBETA, EKZERO, ALPHA, (CORE(K, IC), K=1, 7), OMEGAT, (PHSIG(1), PTALLY60
2  I=1, NEN) PTALLY70
30  NPI=NPI+1 PTALLY80
      RETURN PTALLY90
1500  FORMAT(15H1INITIAL STATE-, 9X2HID, 7X7HNS NP, 6X14HENERGY(PER CM), PTALLYF1
110X10HENERGY(EV)/20X211, 212, 411, 215, F20, 2, 1PE20, 5/14HC OCCUPATIONNP TALLYF2
2- 12X8HALPHA(1), 7X8HALPHA(2), 7X8HALPHA(3), 7X8HALPHA(4), 7X8HALPHA(5PTALLYF3
3), 7X8HALPHA(6)/20X1P6E15, 4/15H0 FINAL STATE-, 7X8HGAMMA(C), 6X4HN(IPTALLYF4
4), 6X4HL(1), 3X7H2S(C)+1, 6X4HL(C), 8X3HFPC, 11X6HK(LIM), 8X8HOMEGA(T)/ PTALLYF5
520X5110, 1P3E15, 4/1H0, 20X19HELECTRON ENERGY(EV), 11X29HPHOPTALLYF6

```

6 TOIONIZATION CROSS SECTION, 15X25HIGH ENERGY CROSS SECTION/ (3E40•4PTALLYF7
7)) PTALLYF8
END PTALLY

```

*   FORTRAN
*   SUBROUTINE PIABS
*   ACCUMULATES PHOTOIONIZATION ABSORPTION COEFFICIENT-
COMMON NOMEA, OMEGA0, DOMEA, NRHO, ALPHAO, TEMP, K1, K2, IGZERO, PICCOMM1
1  NZERO, LZERO, KSZERO, LAZERO, IBETA, EZERO, EKZERO, NS, NP, L12, PICCOMM2
2  IS12, ISPEC, JSPEC, ZRES, ZNUCL, NTOTAL, NIC, ZETANU, OMEGAT, PICCOMM3
3  XNUI, XMUI, XEPI, IGC, NI, LI, ISC, LC, FPSQ, NEN, NPI, NENY,
4  DENS, EDENS, SLIM, PIEDGE, ALPHA, PHSIG, DELEN,
5  SOMEWA, PISIG, PIABS, CORAB
DIMENSION DENS(6), EDENS(6), SLIM(6), PIEDGE(6), ALPHA(6),
1  PHSIG(50), DELEN(50),
2  OMEGA(2000), PISIG(2000), PIABS(2000,6), CORAB(7)
DCI 600 NC=1, NENY
10 READ INPUT TAPE 5, 1000, NOMEA, OMEGA0, DOMEWA
20 DCI 40 N=1, NOMEWA
OMEGA(N)=OMEGA0+FLOATF(N-1)*DOMEWA
DCI 30 J=1,6
30 PIABS(N,J)=0.0
40 CONTINUE
50 READ TAPE 15, NTOTAL, ALPHAO, TEMP, DELEN, NRHO, NEN
DCI 500 LCOUNT=1, NP1
100 READ TAPE 15, K1, K2, IGZERO, NZERO, LZERO, KSZERO, LAZERO, IBETA, PIABS100
1  EKZERO, ALPHA, CORAB, OMEGAT, (PHSIG(I), I=1, NEN)
X=0.0
110 DCI 125 J=1, NRHO
ALPHA(J)=ALPHA(J)*DENS(J)*1.0E-18
IF(SLIM(J) 115, 115, 120
115 PIEDGE(J)=0.0
GO TO 125
120 PIEDGE(J)=13.605*(FLOATF(K2)/SLIM(J))**2
X=MAX1(X, PIEDGE(J))
125 CONTINUE
DCI 300 N=1, NOMEWA
IF(OMEGA(N)-OMEGAT+X) 300, 175, 175
175 DCI 190 I=2, NEN
IF(OMEGA(N)-OMEGAT-DELEN(I)) 200, 200, 190
PIABS 0
PIABS C1
PIABS 1
PIABS 2
PIABS 10
PIABS 20
PIABS 30
PIABS 40
PIABS 50
PIABS 60
PIABS 70
PIABS 80
PIABS 90
PIABS100
PIABS110
PIABS115
PIABS120
PIABS130
PIABS140
PIABS150
PIABS160
PIABS170
PIABS175
PIABS180
PIABS210
PIABS220
PIABS230
PIABS240

```

```

190 CONTINUE
191      I=1
192      PI SIG(N)=PHSIG(I-1)+(OMEGA(N)-OMEGAT- DELEN(I-1))/ (DELEN(I)-
193      DELEN(I-1))* (PHSIG(I)-PHSIG(I-1))
194      IF (PI SIG(N)) 225, 300, 300
195      PI SIG(N)=0.0
196      CONTINUE
197      DO 400 J=1,NRHO
198      IF (CORAB(2)-SLIM(J)) 150, 150, 400
199      IF (ALPHA(J)) 400, 400, 155
200      DO 250 N=1,NOMEGA
201      IF (OMEGA(N)-OMEGAT+PIEDGE(J)) 250, 160, 160
202      PI ABS(N,J)=PIABS(N,J)+ALPHA(J)*PI SIG(N)
203      PIABS(N,J)=PIABS(N,J)+ALPHA(J)*PI SIG(N)
204      CONTINUE
205      CONTINUE
206      CONTINUE
207      REWIND 15
208      CALL ABRITE
209      CONTINUE
210      FORMAT(110,2E20.8)
211      RETURN
212      END

```

```

*   FORTRAN SUBROUTINE ABRITE          ABRIT 0
C   ACCUMULATED ABSORPTION COEFFICIENT PRINTED AND WRITTEN ONTO TAPE A6- ABRIT C1
COMMON NOMEA, OMEGA0, DOMEA, NRHO, ALPHAO, TEMP, K1, K2, IGZERO, PICCOMM1
1  NZERO, LZERO, KSZERO, LAZERO, IBETA, EZERO, EKZERO, NS, NP, L12, PICCOMM2
2  IS12, ISPEC, JSPEC, ZRES, ZNUCL, NTOTAL, NIC, ZETANU, OMEGAT, PICCOMM3
3  XNUI, XMUI, XEPI, IGC, NI, LI, ISC, LC, FPSQ, NEN, NPI, NENY, PICCOM 4
4  DENS, EDENS, SLIM, PIEDGE, ALPHA, PHSIG, DELEN, PICCOM 5
5  OMEGA, PISIG, PIABS, CORAB, PICCOM26
DIMENSION DENS(6), EDENS(6), SLIM(6), PIEDGE(6), ALPHA(6), PICDIM 1
1  PHSIG(50), DELEN(50), PICDIM23
2  OMEGA(2000), PISIG(2000), PIABS(2000,6), CORAB(7)
IF(NOMEA-2000) 50, 100, 100
50 M=NOMEA+1
DO 75 N=M, 2000
OMEGA(N)=0.0
DO 60 J=1, NRHO
60 PIABS(N,J)=0.0
75 CONTINUE
100 WRITE TAPE 16, NOMEA, OMEGA0, DOMEA, OMEGA, PIABS
LC=100
200 DO 300 N=1, NOMEA
E=8065.98*OMEGA(N)
WAVE=12398.1/OMEGA(N)
1F(LC-50) 250, 250, 225
225 WRITE OUTPUT TAPE 6, 1000, TEMP, ALPHAO, NOMEA, OMEGA0, DOMEA
WRITE OUTPUT TAPE 6, 1020
LC=1
250 WRITE OUTPUT TAPE 6, 1030, OMEGA(N), E, WAVE, (PIABS(N,J), J=1,6)
LC=LC+1
300 CONTINUE
RETURN
1000 FORMAT(34H1 CONTINUUM ABSORPTION COEFFICIENT-, 15X1H TEMPERATURE, 12X ABRIT1F1
18ALPHA(0), 4X8HN(OMEGA), 5X8HOMEGA(0), 4X11H DELTA OMEGA/40X, 1PE20.2, ABRIT1F1
2E20.2, 110, 2E15.4)
1020 FORMAT(1H0, 5X, 6H ENERGY, 8X, 6H ENERGY, 5X, 11H WAVE LENGTH, 26X, 32H ABSORPTION ABRIT F3

```

ITION COEFFICIENT (PER CM•) /1H •6X•4H(EV)•9X•6H(1/CM)• 6X•10H(ANGSTABRI T F4
2ROM)•5X•8HALPHA(1)•6X•8HALPHA(2)•6X•8HALPHA(3)•6X•8HALPHA(4)•6X•8HALPHA(5)•6X•8HALPHA(6)•1
3ALPHA(5)•6X•8HALPHA(6)•1
1030 FORMAT(1P9E14•4)
END

```

* FORTRAN
SUBROUTINE PFINIS
COMMON NOMEA, OMEGA0, DOMEA, NRHO, ALPHAO, TEMP, K1, K2, IGZERO, PICCOMM1
1 NZERO, LZERO, KSZERO, LAZERO, IBETA, EZERO, EKZERO, NS, NP, L12, PICCOMM2
2 IS12, ISPEC, JSPEC, ZRES, ZNUCL, NTOTAL, NIC, ZETANU, OMEGAT, PICCOMM3
3 XNU1, XMUI, XEPI, IGC, NI, LI, ISC, LC, FPSQ, NEN, NPI, NENY,
4 DENS, EDENS, SLIM, PIEDGE, ALPHA, PHSIG, DELEN,
5 OMEGA, PISIG, PIABS, CORAB
6 DIMENSION DENS(6), EDENS(6), SLIM(6), PIEDGE(6), ALPHA(6),
7 PHSIG(50), DELEN(50),
8 OMEGA(2000), PISIG(2000), PIABS(2000,6), CORAB(7)
9 REWIND 15
10 PFINIS10
11 PFINIS20
12 PFINIS30
13 PFINIS40
14 PFINIS50
15 PFINIS60
16 PFINIS70
17 PFINIS80
18 PFINIS85
19 PFINIS86
20 PFINIS90
21 PFINIS90
22 PFINI100
23 PFINI110
24 PFINI120
25 PFINI130
26 PFINIS
27
100 CONTINUE
100 END FILE 15
100 CALL UNLOAD(15)
100 CALL UNLOAD(25)
100 RETURN
100 END

```

```

*
* FORTRAN SUBROUTINE PMEAN
COMMON NOMEGA, OMEGA0, DOMEGA, NRHO, ALPHAO, TEMP, K1, K2, IGZERO, PICCOMM1
1 NZERO, LZERO, KSZERO, LAZERO, IBETA, EZERO, EKZERO, NS, NP, L12, PICCOMM2
2 IS12, ISPEC, JSPEC, ZRES, ZNUCL, NTOTAL, NIC, ZETANU, OMEGAT, PICCOMM3
3 XNU1, XMUI, XEPI, IGC, NI, LI, ISC, LC, FPSQ, NEN, NPI, NENY, PICCOMM4
4 DENS, EDENS, SLIM, PIEDGE, ALPHA, PHSIG, DELEN, PICCOMM5
5 PHSIG(50), DELEN(50), PICCOMM6
6 DIMENSION DENS(6), EDENS(6), SLIM(6), PIEDGE(6), ALPHA(6),
7 OMEGA(2000), PISIG(2000), PIABS(2000,6), CORAB(7), PLATM(6),
8 DIMENSION PLANK1(6), PLANK2(6), ACCI(6), VINTE(6)
9 WRITE OUTPUT TAPE 6,299
299 FORMAT(1H1)
TT = TEMP
PP = 3.1415927
PP4 = PP*PP*PP*PP
TT4 = TT*TT*TT*TT
CONST = 15.0/(PP4*TT4)
LAST = NOMEGA -1
DO 30 J=1, NRHO
ACCI(J) = 0.0
30 CONTINUE
DC 100 I = 1, LAST
IF (I-1)60, 50, 60
50 FCONS = EXPF(-OMEGA(I)/TEMP)*(OMEGA(I)**3)
DC 500 J=1, NRHO
PLANK1(J) = PIABS(I,J)*FCONS
500 CONTINUE
60 I = I+1
SCONS = EXPF(-OMEGA(I)/TEMP)*(OMEGA(I)**3)
DO 550 J=1, NRHO
PLANK2(J) = PIABS(I,J)*SCONS
VINTE(J) = (PLANK1(J)+PLANK2(J))*DOMEGA *0.5
ACCI(J) = VINTE(J) + ACCI(J)
PLANK1(J) = PLANK2(J)
PMEAN131

```

550 CONTINUE
100 CONTINUE
DO 33 J=1, NRHO
PLATM(J) = CONST * ACC1(J)
WRITE OUTPUT TAPE 6,300,PLATM(J),J
33 CONTINUE
300 FORMAT(11H PLANK MEAN,5X,E20.8,3H J= 12)
200 CONTINUE
RETURN
END

PMEAN191
PMEAN211
PMEAN221
PMEAN231
PMEAN241
PMEAN251

Appendix D COMPUTER CODES RABS AND ROSS

To provide a calculation of Rosseland mean opacities the computer codes RABS and ROSS have been developed. The code RABS is a modification of MULTIPLET (Appendix B). Input-output information to RABS is provided in Sec. D. 1; a brief description of those subroutines in RABS which differ from MULTIPLET is in Sec. D. 2, a source program listing of these subroutines is provided in Sec. D. 3.

The Rosseland mean calculation is carried out by the code ROSS, using the tape provided by RABS. Input-output information for ROSS is provided in Sec. D. 4; Sec. D. 5 lists the FORTRAN parameters used by the code, their definitions, and their dimensions. Section D. 6 provides a brief description of each subroutine of the code, and a list of the complete source program constitutes Sec. D. 7.

D. 1 INPUT-OUTPUT OF THE CODE RABS

- A. Data cards are read in the following order (FORTRAN FORMAT in parentheses).
 1. Card 1 - NTAG, (I10): NTAG = 2
 2. Card 2 - ABSMIN (E 20.8):
TEMP (E 20.8):
NENGY (I10): } (Card 3 of MULTIPLET,
Appendix B, §1A4)
 3. Card 3 - DENS (1, J) (6E12.6): (Card 4 of MULTIPLET)
 4. Card 4 - DENS (2, J) (6E12.6): (Card 5 of MULTIPLET)
 5. Cards 5 through 14 - PSI2 (8F5.4):
PSI1 (17F4.1):
PSI (17F4.4) (8 cards): } (Cards 6 through 15 of
MULTIPLET)
 6. Card 15 - AB (6E12.6): The six photon energies at which the free-free absorption coefficient is tabulated AB(N) = E_N , (N = 1, 6)

7. Cards 16-21 - CAB (6E12.6) (6 cards): the free-free absorption coefficient at the six densities for each of the six values of the photon energy:

$$\text{CAB}(J, N) = \mu(\text{FREE-FREE}) \text{ at density } J \text{ and energy } E_N = AB(N) \quad (N = 1, 6).$$

8. NENCY - Energy spectrum cards:

(same as MULTIPLET, Appendix B, §1A8)

Must agree with those used in PIC to generate tape used on Tape unit A6.

B. The systems input tape is Tape 5; the systems output tape is Tape 6. Tape 26 (B6) contains the tables of atomic data utilized by MULTIPLET (Appendix B, §1B)

Tape 15 (A5) is the LINE ATLAS generated by MULTIPLET (Appendix B, §1B)

Tape 16 (A6) is the PHOTONIZATION ATLAS and the tables of the accumulated absorption coefficients generated by PIC (Appendix C, §1B)

C. The output listing is identical to that generated by MULTIPLET (Appendix B, §1C).

D. 2 THE RABS FORMULA SET

Common and Dimensions agree with MULTIPLET (Appendix B, §2).

A. MAIN PROGRAM

1. If NTAG = 0, 1: Calls EXIT
2. If NTAG = 2: Calls MSET, calls modified version of MULTIPLET III (the subroutines RABS, FINIS)

B. ABS: A dummy routine to replace the ABS routine of MULTIPLET

C. RABS: A modification of the routine ABS of MULTIPLET (see Appendix B, §III D 1)
The free-free absorption coefficient is read from cards. For each table of the absorption coefficient (NENCY tables in all): the corresponding

tabulated photoionization absorption coefficient generated by code PIC is read from the second file of the tape on Tape Unit A6. The free-free absorption coefficient is interpolated to the energies OMEGA (N) and added to the photoionization absorption coefficient. Transitions are then read from the LINE ATLAS one at a time. If the line is a weak narrow line it is ignored; if the line is a strong narrow line the line wings are accumulated with the tabulated absorption coefficient. (The distinction between strong and weak narrow lines is defined in Sec. 6). The broad lines are accumulated as in MULTIPLET.

D. The following subroutines must be provided and are identical to the routines in MULTIPLET.

1. MULTIPLET I

ENSORT

O

P

Q2

S2

S12

FPC

U

W

SF

BSORT

ORDER

LIST

ASORT

TWRITE

2. MULTIPLET II

MSET

TREAD

ATLAS

FCALC

SLATER

FHYDRO

WIDTH

3. MULTIPLET III

VOIGT

TALLY

FINIS

MEAN

D. 3 LIST OF SOURCE PROGRAM OF RABS

C MULTIPLET- MAIN PROGRAM- ROSSELAND VERSION

```

* FORTRAN
COMMON J1,J2,J3,J4,J5,J6,J7,J1P,J2P,J3P,J4P,J5P,J6P,J7P,IBETA,
1 NCASE,ALPHAO,ALPHA, E, ID1, ID2, B,NREC, LTOT, NTOT,NDIM
DIMENSION ALPHA(1500,6),E(1500),ID1(1500),ID2(1500),B(1500,3)
REWIND 15
REWIND 16
REWIND 25
REWIND 26
NDIM=1500
READ INPUT TAPE 5, 1000, NTAG
IF(NTAG) 10, 10, 200
10 READ INPUT TAPE 5, 1010, NCASE, ALPHAO
IF(NCASE-NDIM) 50, 50, 20
20 WRITE OUTPUT TAPE 6, 1015, NCASE
CALL EXIT
50 IF(NCASE-1) 60, 60, 70
60 WRITE OUTPUT TAPE 6, 1020, NCASE
CALL EXIT
70 READ INPUT TAPE 5, 1025, (ID1(I), ID2(I), IBETA, E(I), (ALPHA(I,J),
1 J=1,6), I=1,NCASE)
CALL ENSORT(NCASE)
C WRITE INPUT DATA
80 LC=100
DO 100 K=1,NCASE
100 IF(LC-50) 90, 90, 85
85 WRITE OUTPUT TAPE 6, 1030, NCASE, ALPHAO,IBETA
LC=1
90 WRITE OUTPUT TAPE 6, 1040, K, ID1(K), ID2(K), E(K), (ALPHA(K,J),
1 J=1,6)
LC=LC+1
100 CONTINUE
CALL EXIT
CALL ORDER
CALL TWRITE
REWIND 25

```

```

REWIND 15
200 CALL NSET
NTAG=NTAG+1
GO TO( 210, 300, 350),NTAG
210 CALL ATLAS
300 CALL ABS
GO TO 400
350 CALL RABS
400 CALL FINIS
401 CALL UNLOAD(26)
CALL EXIT
1000 FORMAT( 110)
1010 FORMAT( 110,E10.8)
1015 FORMAT(16H1TOO MANY STATES,110)
1020 FORMAT(15H1TOO FEW STATES,110)
1025 FORMAT(14,I5,I1,E10.8,6E8.6)
1030 FORMAT( 28H1MULTIPL ET DATA LIST- NCASE=I4,I3H
1 4X,6H BETA=I4/I14HO 1
2HA(1) ALPHA(2) ALPHA(3) ALPHA(4)
3A(6)// )
1040 FORMAT(15,I15,I5,1P7E13.5,/)
END
MULT 320
MULT 330
MULT 340
MULT 341
MULT 350
MULT 360
MULT 361
MULT 362
MULT 370
MULT 380
MULT 390
MULT F2
MULT F3
MULT F4
MULT F5
MULT F6
ALPHA(0)=E14.6,3HMP
ENERGY ALPMMP
ALPHA(5) ALPHMP
MP F6
MP F7
MP E

```

```
      SUBROUTINE ABS
      SUBROUTINE ABS
      NTAG=2
      WRITE OUTPUT TAPE 6,1,NTAG
      1 FORMAT (1H0,3X,7HNTAG = 13)
      RETURN
      END
```

```

0
FORTRAN
FORTRAN
      SUBROUTINE RABS
      EVALUATE ABSORPTION COEFFICIENT DUE TO BROAD LINES IN LINE ATLAS-
      NARROW LINES ACCUMULATED FOR ROSELAND MEAN CALCULATION-
      COMMON ABSMIN, TEMP, NENGY, DENS, NSLIM, NMAX, WFACT, LTOT, K1, K2, MULT
      1  ICI, NI, LI, KSI, LAI, NSI, NPI, L121, IS121, IGF, NF, LF, KSF, MULT
      2  LAF, NSF, NPF, L12F, IS12F, DELTAE, Z, ALPHA, FNO, SIGSQ, GFACT, MULT
      3  WCOLL, WDOPP, EI, XMCSQ, DENMIN, NMAX, MULT
      4  NOMEA, OMEGA0, DOMEA, OMEGA, ABS, PSI1, PSI2, PSI
      DIMENSION DENS(2,6), NSLIM(6), ALPHA(6), CAB(6,6), RHOAB(6),
      1  OMEGA(2000), ABS(2000,6), AB(6), PSI1(17), PSI2(8), PSI(17,8)
      REWIND 15
      REWIND 16
      REWIND 25
      READ INPUT TAPE 5, 1500, PSI12, PSI1, PSI
      GO TO 700
      10  DO 600 NEN=1, NENGY
      20  READ INPUT TAPE 5, 1000, NOMEA, OMEGA0, DOMEGA
      READ TAPE 16, NOMP, OMP, DOMP, OMEGA
      DO 25 J=1,6
      25  READ TAPE 16, (ABS(N,J), N=1,2000)
      IF (NOMP-NOMEA) 30, 35, 30
      30  WRITE OUTPUT TAPE 6, 1640, NOMP, NOMEA, OMP, OMEGA0, DOMP, DOMEGA
      CALL EXIT
      35  IF (OMP-OMEGA0) 30, 40, 30
      40  IF (DOMP-DOMEGA) 30, 800, 30
      50  READ TAPE 15, LTOT, NCASE, ALPHA0, IBETA
      NCENT=2
      100  DO 500 LCOUNT=1,LTOT
      READ TAPE 15, DELTAE, Z, FNO, SIGSQ, GFACT, WCOLL, WDOPP, ID11,
      1  ID21, EI, ID1F, ID2F, ALPHA, XMCSQ
      K1P=ID11/1000
      IF (K1P-K1) 110, 120, 110
      110  WRITE OUTPUT TAPE 6, 1650, K1P, K1
      CALL EXIT

```

```

120 IF(OMEGA0-DELTAE) 140, 130, 130
130 OMEGAC=DELTAE
N=1
140 IFLAG=1
GO TO 200
140 DO 150 N=NCENT, NOMEGA
IF(OMEGA(N)-DELTAE) 150, 160, 160
150 CONTINUE
OMEGAC=DELTAE
N=NOMEGA
NCENT=N
IFLAG=0
GO TO 200
160 IF(OMEGA(N)-DELTAE-ABSF(DELTAE-OMEGA(N-1))) 170, 170, 180
170 OMEGAC=OMEGA(N)
NCENT=N
GO TO 190
180 OMEGAC=OMEGA(N-1)
NCENT=N-1
N=N-1
190 IFLAG=0
200 DO 400 J=1,6
IF(ALPHA(J) 400, 400, 210
210 ALPHA(J)=ALPHA(J)*DENS(1,J)
Y=WCOLL*DENS(2,J)*10.0
220 IF(2.0*Y-DOMEGA) 230, 240, 240
230 IF(OMEGA0-DELTAE) 232, 232, 240
232 IF(OMEGA(NOMEGA)-DELTAE) 240, 235, 235
235 S=ALPHA(J)/3.14159*FNO/Y
IF(S-0.5*(ABS(N+1,J)+ABS(N,J)) 400, 236, 236
236 OMEGAC=DELTAE
IF(OMEGAC-OMEGA(NCENT)) 237, 238, 238
237 NCENT=NCENT-2
NCENT=NCENT+1
GO TO 240
238 N=NCENT-1
NCENT=NCENT+2
RABS 444
RABS 450
RABS 451
RABS 452
RABS 453

```

```

240 NQ=N
  IQ=IFLAG
  ETA=WDOPP/Y
  250 X=(OMEGA(NQ)-OMEGAC)/Y
  IF(ETA-0.2) 280, 280, 260
  260 IF(ABSF(X)/ETA-5.0) 270, 280, 280
  270 B=1.0/(3.14159*Y)*VOIGT(X,ETA,Y)
  GO TO 300
  280 B=1.0/(6.28318*Y)*(1.0/(1.0+(X+0.7071*ETA)**2)+1.0/(1.0+(X-
  1 *7071*ETA)**2))
  300 XABS=ALPHAI(J)*FNO*B
  IF(XABS-ABSMIN*ABS(NQ,J)) 310, 330, 330
  310 IF(IQ) 320, 320, 400
  320 NQ=NCENT
  IQ=1
  GO TO 340
  330 ARS(NQ,J)=ARS(NQ,J)+XARS
  IF(IQ) 350, 350, 340
  340 NQ=NQ+1
  IF(NQ-OMEGA) 250, 250, 400
  350 NQ=NQ-1
  IF(NQ) 320, 320, 250
  400 CONTINUE
  500 CONTINUE
  REWIND 15
  DO 510 J=1,6
  510 AB(J)=15399/TEMP**4*AB(J)
  WRITE OUTPUT TAPE 6, 1200, OMEGA0,OMEGA,OMEGA(INOMEGA),AB
  CALL TALLY
  600 CONTINUE
  RETURN
  700 READ INPUT TAPE 5, 1600, AB, CAB
  710 WRITE OUTPUT TAPE 6, 1610, TEMP, (DENS(1,J), DENS(2,J), J=1,6)
  720 READ TAPE 16, NTOT, ALPH, T,(X,J=1,50), NRHO, NEN
  IF(T-TEMP) 725, 730, 725
  ABS 46
  ABS 47
  ABS 49
  ABS 48
  ABS 50
  ABS 51
  ABS 52
  ABS 53
  ABS 54
  ABS 55
  ABS 56
  ABS 57
  ABS 58
  ABS 59
  ABS 60
  ABS 61
  ABS 62
  ABS 63
  ABS 64
  ABS 65
  ABS 66
  ABS 67
  ABS 68
  ABS 69
  ABS 70
  ABS 71
  ABS 72
  ABS 73
  ABS 74
  ABS 75
  ABS 76
  RABS7000
  RABS7010
  RABS7020
  RABS7030

```

```

725 WRITE OUTPUT TAPE 6, 1620, T, TEMP
    CALL EXIT
730 READ TAPE 16, K1
    CALL SFIL(16,1)
740 READ TAPE 16, NENP
    IF(NENP-NENY) 745, 10, 745
745 WRITE OUTPUT TAPE 6, 1630, NENP, NENY
    CALL EXIT
C EVALUATE FREE-FREE AND COMPTON ABSORPTION COEFFICIENTS-
    800 DO 810 J=1,6
    810 RHOAB(J)=DENS(2,J)*.6654E-24
    DO 850 N=1,NOMEGA
    IF(OMEGA(N)-AB(6)) 820, 830, 830
820 DO 825 K=1,6
    IF(OMEGA(N)-AB(K)) 840, 840, 825
825 CONTINUE
830 DO 835 J=1,6
    ABS(N,J)=ABS(N,J)+CAB(J,K+1)*(AB(6)/OMEGA(N))**3+
    1 RHOAB(J)/(1.0-EXP(-OMEGA(N)/TEMP))
835 CONTINUE
    GO TO 850
840 DO 845 J=1,6
    ABS(N,J)=ABS(N,J)+CAB(J,K)+(OMEGA(N)-AB(K))/(AB(K+1)-AB(K))-
    1 (CAB(J,K+1)-CAB(J,K))+RHOAB(J)/(1.0-EXP(-OMEGA(N)/TEMP))
845 CONTINUE
850 CONTINUE
    GO TO 50
1000 FORMAT(110, 2E20.8)
1200 FORMAT(42H1 NARROW LINE CONTRIBUTION TO PLANCK MEAN-, 20X, 7HENERGY=ABS
1.1PE9*3, 1H(.1PE9*3, 1H), 1PE9*3/6E20.6)
1500 FORMAT(8F5.4/17F4.1/(17F4.4))
1600 FORMAT(6E12.6)
1610 FORMAT(28H1ROSSELAND LINE CALCULATION-, 10X, 12HTEMPERATURE=1PE12.4, RABS
16H (EV.1/19X, 24HION DENSITY(*1.0975E-16), 14X, 16HELECTRON DENSITY/( RABS
21P2E30.4)
1620 FORMAT(20H1INCORRECT PIC TAPE-, 10X, 11HTEMPERATURE, 10X, 2E20.8)
    RABS F6

```

1630 FORMAT(20H1)INCORRECT PIC TAPE-,10X,5HENERGY,10X,2110,
1640 FORMAT(20H1)INCORRECT PIC TAPE-,10X,15HENERGY SPECTRUM,10X,2110.,/
1 4E20.8
1650 FORMAT(20H1)INCORRECT PIC TAPE-,10X,10HELEMENT ID,10X,2110)
END
RABS F7
RABS F8
RABS F8
RABS F9
ABS

D.4 INPUT-OUTPUT TO THE CODE ROSS

A. Data cards are read in the following order: (FORTRAN FORMAT in parentheses)

1. Card 1 - NENCY, (I10): Number of different tables of the accumulated absorption coefficient. (must agree with PIC value)
K1, (I10): K1 = 0, oxygen; K1 = 1, nitrogen.
IBETA, (I10): temperature index
TEMP, (E20.8): kT (in eV)
2. Card 2 - RHOI, (6E12.8): Ion densities (particles/cm³) at the 6 densities (J = 1, 6).
3. Card 3 - RHOE, (6E12.8): Electron densities (particles/cm³) at the 6 densities (J = 1, 6).

B. Two versions of ROSS are currently used: one for the calculation of the Rosseland mean opacity of the nitrogen-oxygen mixture in air and one for the Rosseland calculation of pure nitrogen or oxygen.

1. Air calculation - the LINE ATLAS tapes for oxygen and nitrogen generated by the code RABS are on Tape Units 15(A5) and 16(A6). An air LINE ATLAS is generated from these and written onto Tape Unit 25 (B5).
2. Nitrogen (or oxygen) calculation - the LINE ATLAS tape generated by the code RABS is on Tape Unit 25 (B5).

C. The Output Listing

1. The total mean free path (cm) averaged over frequency interval $\Delta\omega$ for the six densities at the energies $\epsilon_N = \omega_0 + (N - 1)\Delta\omega$, (N = 1, N_ω). (written by subroutine XMFP).
2. The partial Rosseland mean free path (cm) integrated from ω_0 to $\epsilon_N = \omega_0 + (N - 1)\Delta\omega$ is tabulated as a function of ϵ_N for the six densities

Note Items 1 and 2 are repeated NENCY times, once for each portion of the energy spectrum designated by one NENCY card in code PIC.

D. 5 DEFINITIONS OF PARAMETERS IN COMMON STORAGE

Dimensions of dimensioned variables are given in parentheses.

NENGY	Number of tables of the absorption coefficient
OMEGA	(2000): photon energies at which the absorption coefficient is tabulated. $\text{OMEGA}(N) = \omega_0 + (N - 1)\Delta\omega$, ($N = 1, N_\omega$)
NOMEGA	N_ω : number of photon energies at which the absorption coefficient is tabulated
OMEGA0	ω_0 : lowest photon energy at which the absorption coefficient is tabulated
DOMEGA	$\Delta\omega$: interval in the photon energy table
ABS	(2000×6): $\text{ABS}(N, J) = \text{total absorption coefficient (cm}^{-1}\text{) at energy } \epsilon_N = \text{OMEGA}(N)$, density J .
RHOI	(6): $\text{RHOI}(J) = \text{number ions/cm}^3$ at density J , ($J = 1, 6$)
RHOE	(6): $\text{RHOE}(J) = \text{number electrons/cm}^3$ at density J , ($J = 1, 6$)
LDIM	Parameter defining dimension of array OMEGA (LDIM = 2000)
KDIM	Parameter defining the maximum number of lines allowed in an interval $3(\Delta\omega)$
WC	(6): Working storage
IBETA	β : temperature index
TEMP	kT in eV
K1	$K1 = 0$, oxygen; $K1 = 1$, nitrogen

D. 6 THE ROSS FORMULA SET

A. MAIN PROGRAM

1. The input data are read and the density values are listed.
2. If an air calculation calls AIR to generate from Tapes A5 and A6 an air tape on Unit B5.

3. Calls ACCUM(N) to read the N^{th} table of the accumulated absorption coefficient from the second file of Tape B5.
4. Calls XMFP to evaluate the mean free path as a function of energy and density.
5. Calls RMEAN to evaluate the Rosseland mean opacity, as a function of energy and density, from the mean free path generated by XMFP.

Items 3, 4, and 5 are repeated NENCY times, once for each table of the absorption coefficient.

B. AIR

The LINE ATLAS tapes for nitrogen and oxygen are mounted on Tape Units A5 and A6. The line-transition data are read one line at a time from these two tapes and written in order of increasing energy onto an air tape on Tape Unit B5. The nitrogen occupation numbers ALPHA are multiplied by (0.78823) and the oxygen numbers by (0.21177). The tables of the accumulated absorption coefficients for nitrogen and oxygen are combined (nitrogen values multiplied by 0.78823, oxygen values multiplied by 0.21177) and written onto Tape B5. Tapes A5 and A6 are unloaded and Tape B5 is rewound.

C. ACCUM(N)

The N^{th} table of the accumulated absorption coefficient is read from the second file of Tape B5. Tape B5 is rewound.

D. XMFP

XMFP evaluates the radiative mean free path averaged over the frequency interval $\Delta\omega$ for each value of the photon energy and each value of the

density. For each energy ϵ_N ($N = 1, N_\omega$) the LINE ATLAS on Tape Unit B5 is searched for all narrow lines lying in the frequency interval $(\epsilon_{N-1}, \epsilon_{N+2})$. Each line found is classified as strong or weak by comparison with the accumulated absorption coefficient due to broad lines plus continuum contributions - averaged over the frequency interval $\Delta\omega$. Each weak line (line center ϵ_c , width w) is assumed to have a rectangular line shape, and the interval $\Delta\omega$ is subdivided at the frequencies $\epsilon_\pm = (\epsilon_c \pm w)$. Each strong line is assumed to have a Lorentz line shape, and the interval $\Delta\omega$ is subdivided at the frequencies $E_n = \left[\epsilon_c \pm 2n\left(\frac{w}{2}\right) \right]$, ($n = 0, \dots$ such that $\epsilon_N < E_n < \epsilon_{N+1}$). When all narrow lines in the frequency interval $(\epsilon_{N-1}, \epsilon_{N+2})$ have been found the frequencies E (for weak and strong lines, i.e., E_\pm, E_n) which subdivide $\Delta\omega$ constitute a set of energies adequate to represent all the narrow lines in $\Delta\omega$. The absorption coefficient in $(\epsilon_N, \epsilon_{N+1})$ due to the narrow lines in $(\epsilon_{N-1}, \epsilon_{N+2})$ is then evaluated at each of the frequencies E and accumulated with the absorption coefficient due to broad lines and continuum contributions. The mean free path, averaged over $\Delta\omega$, is then evaluated by numerical integration and is listed.

E. RMEAN

The Rosseland mean free path [Eq. (6.2)] is evaluated at each density J and each energy $\epsilon_N = \text{OMEGA}(N)$ ($N = 1, N_\omega$) by numerical integration of the mean free path obtained by XMFP from ω_0 to ϵ_N . The resulting partial Rosseland mean free paths are listed.

D. 7 LIST OF SOURCE PROGRAM OF ROSS

```

* FORTRAN
C MAIN PROGRAM ROSS- TO EVALUATE ROSSELAND MEAN OPACITIES-
COMMON NE:NGY, OMEGA, NOMEGA, DOMEAO, ABS, RHOI, RHOE,
1 LDIM, KDIM, WC, IBETA, TEMP, K1
DIMENSION OMEGA(2000), ABS(2000,6), RHOI(6), RHOE(6),WC(6)
CALL AIR
READ INPUT TAPE 5, 1000, NENGY, K1, IBETA, TEMP
REWIND 25
READ INPUT TAPE 5, 1010, RHOI, RHOE
WRITE OUTPUT TAPE 6, 1020, TEMP, (RHOI(J),RHOE(J),J=1,6)
DO 100 N=1,NENGY
CALL SFIL(25,1)
CALL ACCUM(N)
CALL XMFP
CALL RMEAN
100 CONTINUE
CALL UNLOAD(25)
CALL EXIT
1000 FORMAT(3110,E20.8)
1010 FORMAT(6E12.8)
1020 FORMAT(28H1ROSSELAND MEAN CALCULATION-10X,12HTEMPERATURE=1PE12.4,6ROSS
1H (EV.)//19X11HION DENSITY,14X,16HELECTRON DENSITY/(1P2E30.4))
END

```

* FORTTRAN

SURROUTINE AIR
COMMON NENGY,OMEGA,OMEGA0,DOMEGA,ABS

COMMON A,IDI,B,JDJ,C,XM

DIMENSION OMEGA(20000),ABS(2000,6),ALPHA(6)

DIMENSION A(7,2),IDI(2,2),B(2,2),JDJ(2,2),C(6,2),XM(2)

REWIND 15

REWIND 16

REWIND 25

READ TAPE 15,LTOT1,NCASE1,ALPHAO,IBETA1

READ TAPE 16,LTOT2,NCASE2,ALPHAO,IBETA2

IF (IBETA1-IBETA2) 5,10,5

5 WRITE OUTPUT TAPE 6,1000,IBETA1,IBETA2

1000 FORMAT(23H1WRONG TEMPERATURE I1=I2,3X,3H12=I2)

GO TO 500

10 LTOT=LTOT1+LTOT2

NCASF=NCASE1+NCASE2

WRITE TAPE 25,LTOT,NCASE,ALPHAO,IBETA1

L1=1

L2=1

M=1

M1=0

M2=0

READ TAPE 15,(A(I,1),I=1,7),IDI(1,1),IDI(2,1),B(1),IDJ(1,1),

1IDJ(2,1),(C(J,1),J=1,6),XM(1)

READ TAPE 16,(A(I,2),I=1,7),IDI(1,2),IDI(2,2),B(2),IDJ(1,2),

1IDJ(2,2),(C(J,2),J=1,6),XM(2)

160 IF(A(1,1)-A(1,2)) 20,20,30

20 N=15

K=1

GO TO 40

30 N=16

K=2

40 K1=IDI(1,K)/1000

IF(K1-1) 50,60,60

50 F=0,21177

```

GO TO 70
60  F=0.7882?
70  DO 80  J=1,6
80  C(J,K)=C(J,K)*F
      WRITE TAPE 25,(A(I,K),I=1,7),IDI(1,K),IDI(2,K),B(K),IDJ(1,K),
11D(J(2,K),C(J,K),J=1,6),XM(K)
      GO TO 90,100),K
90  IF(L1-LTOT1) 110,120,120
110 L1=L1+1
      READ TAPE 15,(A(I,1),I=1,7),IDI(1,1),IDI(2,1),B(1),IDJ(1,1),
11D(J(2,1),C(J,1),J=1,6),XM(1)
      GO TO 130
120 M1=1
      GO TO 170
100 IF(L2-LTOT2) 140,150,150
140 L2=L2+1
      READ TAPE 16,(A(I,2),I=1,7),IDI(1,2),IDI(2,2),B(2),IDJ(1,2),
11D(J(2,2),C(J,2),J=1,6),XM(2)
      GO TO 130
150 M2=2
170 M=M1+M2+1
130 GO TO (160,30,20,200),M
200 IF(L1+L2-LTOT) 210,220,220
210 WRITE OUTPUT TAPE 6,1100,M,M1,M2,L1,LTOT1,L2,LTOT2,A(1,1),A(1,2),
1A(1,K)
1100 FORMAT(23H1ERROR--UNFINISHED TAPE/,3H M=12,3X,3HM1=12,3X,3HM2=12,3
1X,3HL1=15,6X,6HLTOT1=15,6X,3HL2=15,6X,6HLTOT2=15,6H DELL1=1PE10,3,
26X,5HDFL2=E10,3,6X,4HDEL=E10,3)
500 END FILE 25
501 CALL UNILCAD(15)
      CALL UNLOAD(16)
      CALL UNLOAD(25)
      CALL EXIT
220 END FILE 25
      REWIND 15
      REWIND 16

```

```

REWIND 25
CALL SFIL(15,1)
CALL SFIL(16,1)
CALL SFIL(25,1)
C READ SECOND FILE
1FIN-15) 230,230,240
230 F1=F
F2=1.0-F
GO TO 250
240 F1=1.0-F
F2=F
250 READ TAPE 15,NEN1
READ TAPE 16,NEN2
IF(NEN1-NEN2) 260,270,260
260 WRITE OUTPUT TAPE 6,1200,NEN1,NEN2,F1,F2
1200 FORMAT(21H1ERROR--NENGY UNEQUAL//4H N1=14,6X,3HN2=14,6X,3HF1=1PE10
1*3,6X,3HF2=F10.3)
GO TO 501
270 WRITE TAPE 25,NEN1
DO 340 J=1,NEN1
READ TAPE 15,NOM1,OM1,DOM1,OMEGA
READ TAPE 16,NOM2,OM2,DOM2,OMEGA
IF(NOM1-NOM2) 280,290,280
280 IF(OM1-OM2) 280,300,280
300 IF(DOM1-DOM2) 280,310,280
280 WRITE OUTPUT TAPE 6,1300,NOM1,OM1,DOM1,NOM2,OM2,DOM2
1300 FORMAT(24H1ERROR--TABLES NOT ALIKE//(110,1P2E20.4))
GO TO 501
310 WRITE TAPE 25,NOM1,OM1,DOM1,OMEGA
DO 320 I=1,6
READ TAPE 15, (ABS(K,I),K=1,2000)
READ TAPE 16, (OMEGA(K),K=1,2000)
DO 330 K=1,2000
330 ABS(K,I)=F1*ABS(K,I)+F2*OMEGA(K)
WRITE TAPE 25,(ABS(K,I),K=1,2000)
320 CONTINUE

```

340 CONTINUE
END FILE 25
CALL UNLOAD(15)
CALL UNLOAD(16)
REWIND 25
RETURN
END

```

*   FORTRAN
*   SUBROUTINE ACCUM(N)
C   TO READ CONTINUOUS ABSORPTION COEFFICIENTS FROM LINE TAPE-
C   COMMON NENGY, OMEGA, NOMEAO, OMEGA0, DOMEGA, ABS, RHOI, RHOE,
1   LDIM, KDIM, WC, IBETA, TEMP, K1
1   DIMENSION OMEGA(2000), ABS(2000,6), RHOI(6), RHOE(6), WC(6)
1   IF(N-NENGY) 50, 50, 20
20  WRITE OUTPUT TAPE 6, 1000, N, NENGY
      CALL EXIT
50  READ TAPE 25, NEN
      IF(NEN-NENGY) 60, 70, 60
60  WRITE OUTPUT TAPE 6, 1100, NEN, NENGY
      CALL EXIT
70  DO 100 L=1,N
      READ TAPE 25, NOMEAO, OMEGA0, DOMEGA, OMEGA
DO 80  J=1,6
80  READ TAPE 25, (ABS(K,J),K=1,2000)
100  CONTINUE
      REWIND 25
      RETURN
1000 FORMAT(22H1N GREATER THAN NENGY-->2110)
1100 FORMAT(23H1WRONG ENERGY SPECTRUM-->2110)
      END
      ACCUM 0
      ACCUM C1
      ROSSCOM1
      ROSSCOM2
      ROSSDIM1
      ROSSDIM2
      ACCUM 10
      ACCUM 10
      ACCUM 20
      ACCUM 20
      ACCUM 30
      ACCUM 40
      ACCUM 50
      ACCUM 60
      ACCUM 70
      ACCUM 80
      ACCUM 90
      ACCUM100
      ACCUM110
      ACCUM120
      ACCUM130
      ACCUM140
      ACCUM F1
      ACCUM F2
      ACCUM

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* FORTRAN
* SURROUTINE XMFP
C EVALUATE AVERAGE MEAN FREE PATH-
C COMBINATION NENGY, OMEGA, NOMEA, OMEGA0, DOMEGA, AUS, RHOI, RHOE,
1 LDIM, KDIM, WC, IBETA, TEMP, K1
1 DIMENSION OMEGA(2000), ABS(2000,6), RHOI(6), RHOE(6), WC(6),
1 XABS(2000), DE(200), S(200,6), W(200,6), ALPHA(6), EPS(2000)
LCD=-1
EMIN= 0.0
DOM2=DOMEGA/2.0
REWIND 25
READ TAPE 25, LTOT, NCASE, ALPHAO, IBETAP
IF(IIBETAP-IBETA) 10, 20, 10
10 WRITE OUTPUT TAPE 6, 5045, IBETA, IBETAP
CALL EXIT
20 LDIM=2000
KDIM=200
LTAPE=1
KT=0
NOM=NOMEA-1
DO 500 N=1,NOM
ENL=OMEGA(N)-DOMEGA
ENU=OMEGA(N+1)+DOMEGA
50 IF(LTAE-LTOT) 100, 100, 200
100 READ TAPE 25, DELTAE,Z,FNO,SIGSQ,GFACT,WCOLL,WDOPPP,IDL1,IDL21,EL
1 ID1F, ID2F, ALPHA, XMCSQ
103 IF(DELTAE-ENL) 190, 105, 105
105 IF(DELTAE-ENU) 110, 110, 107
107 BACKSPACE 25
GO TO 200
110 ITA6=0
DO 130 J=1,6
111 IF(ALPHA(J)-ALPHAO) 125, 125, 115
115 WC(J)=RHOE(J)*WCOLL*10.0
116 IF(WC(J)-DOM2) 120, 120, 125
120 ITAG=1

```

```

ALPHA(J)=ALPHA(J)*RHCI(J)*1.09752E-16
50 TO 130
125 ALPHA(J)=0.0
130 CONTINUE
131 IF(ITAG) 190, 190, 135
135 KT=KT+1
136 IF(KT-KDIM) 140, 140, 138
138 WRITE OUTPUT TAPE 6, 5000, DELTAE, N, KT
GO TO 190
140 DE(KT)=DELTAE
DO 170 J=1,6
141 IF(ALPHA(J)) 145, 145, 150
145 S(KT,J)=0.0
GO TO 170
150 S(KT,J)=ALPHA(J)/3.14159*FNO/WC(J)
W(KT,J)=WC(J)
151 IF(S(KT,J)-0.5*(ABS(N+1,J)+ABS(N,J))) 170, 160
160 S(KT,J)=-S(KT,J)
170 CONTINUE
170 LTAPE=LTAPE+1
190 GO TO 50
200 IF(KT) 250, 250, 800
250 DO 300 J=1,6
300 ABSIN,J)=LOGF(ABS(N+1,J)/ABS(N,J)) / (ABS(N+1,J)-ABS(N,J))
GO TO 500
500 IF(LCD) 900, 810, 810
810 IF(OMEGA(N)-EMIN) 900, 820, 820
820 WRITE OUTPUT TAPE 6, 6000, (DE(K), (S(K,J), J=1,6), (W(K,J), J=1,6),
1 K=1,KT)
1000 FORMAT(8H0DBG 1-, (7E15.4/6E15.4/1))
LCD=LCD-1
900 DO 3500 J=1,6
1000 L=2
EPS(1)=OMEGA(N)
EPS(2)=OMEGA(N+1)
DO 1300 K=1,KT

```

```

1025 IF(SIK,J) 1100, 1300, 1025
C WEAK LINE ENERGIES INTO ENERGY TABLE-
1025 X=DE(K)-W(K,J)
Y=DE(K)+W(K,J)
1030 IF(X-OMEGA(N)) 1030, 1060, 1060
1030 IF(Y-OMEGA(N)) 1300, 1035, 1035
1035 L=L+1
1040 IF(L-LDIM) 1040, 1040, 1050
1040 EPS(L)=Y
1040 GO TO 1300
1050 WRITE OUTPUT TAPE 6, 5035, L,N,J,OMEGA(N),SIK,J,DE(K)
1050 GO TO 1300
1060 IF(X-OMEGA(N+1)) 1065, 1065, 1300
1065 L=L+1
1070 IF(L-LDIM) 1070, 1070, 1050
1070 EPS(L)=X
1070 IF(Y-OMEGA(N+1)) 1035, 1035, 1300
C STRONG LINE ENERGIES INTO ENERGY TABLE-
1100 Z=0.5*W(K,J)
1125 Y=DE(K)+Z
1125 IF(DE(K)-OMEGA(N)) 1125, 1150, 1150
1130 Z=2.0*Z
1130 GO TO 1125
1135 IF(Y-OMEGA(N+1)) 1140, 1140, 1300
1135 IF(DE(K)-OMEGA(N+1)) 1145, 1145, 1050
1140 L=L+1
1140 IF(L-LDIM) 1145, 1145, 1050
1145 EPS(L)=Y
1145 GO TO 1130
1150 IF(DE(K)-OMEGA(N+1)) 1225, 1225, 1200
1200 X=DE(K)-Z
1200 IF(X-OMEGA(N+1)) 1210, 1210, 1205
1205 Z=2.0*Z
1205 GO TO 1200
1210 IF(X-OMEGA(N)) 1300, 1215, 1215
1215 L=L+1

```

```

XMF P 640
XMF P C2
XMF P 650
XMF P 660
XMF P 670
XMF P 680
XMF P 690
XMF P 700
XMF P 710
XMF P 720
XMF P 730
XMF P 740
XMF P 750
XMF P 760
XMF P 770
XMF P 780
XMF P 790
XMF P C3
XMF P 800
XMF P 810
XMF P 820
XMF P 830
XMF P 840
XMF P 850
XMF P 860
XMF P 870
XMF P 880
XMF P 890
XMF P 900
XMF P 910
XMF P 920
XMF P 930
XMF P 940
XMF P 950
XMF P 960
XMF P 970

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```

1220 IF(L-LDIM) 1220, 1220, 1050
1220 EPS(L)=X
1220 GO TO 1205
1225 L=L+1
1225 IF(L-LDIM) 1230, 1230, 1050
1230 EPS(L)=DE(K)
1230 Y=DE(K)+Z
1232 X=DE(K)-Z
1232 IF(Y-OMEGA(N+1)) 1235, 1235, 1210
1235 L=L+1
1235 IF(L-LDIM) 1240, 1240, 1050
1240 EPS(L)=Y
1240 IF(X-OMEGA(N)) 1130, 1250, 1250
1250 L=L+1
1250 IF(L-LDIM) 1260, 1260, 1050
1260 EPS(L)=X
1260 Z=2.0*Z
1260 GO TO 1232
1300 CONTINUE
1300 LT=L
1400 IF(LT-2) 1450, 1450, 1500
1450 ABS(N,J)=LOGF(ABS(N+1,J)/ABS(N,J))/(ABS(N+1,J)-ABS(N,J))
1450 GO TO 3500
1500 LTP=LT-1
1500 DO 1550 I=1,LTP
1500 K=I+1
1500 DO 1540 J=K,LT
1500 IF(EPS(I)-EPS(J)) 1540, 1540, 1520
1520 X=EPS(I)
1520 EPS(I)=EPS(J)
1520 EPS(J)=X
1520 CONTINUE
1540 CONTINUE
1550 CONTINUE
1550 IF(LCD) 1900, 1560, 1560
1560 IF(OMEGA(N)-FMIN) 1900, 1570, 1570
1570 WRITE OUTPUT TAPF 6, 6010, (EPS(L),L=1,LT)
1570 DBUG1302

```

```

6C10 FORMAT(8H0DEBUG 2--,(6E20.8))
1930 DU 1910 L=1,LT
1910 XABS(L)=ABS(N,J)+(EPS(L)-OMEGA(N))/DCMEGA*(ABS(N+1,J)-ABS(N,J))
1F1LCD) 2000, 1920, 1920
1920 IF(OMEGA(N)-EMIN) 2000, 1930, 1930
1930 WRITE OUTPUT TAPE 6, 6020, (XABS(L),L=1,LT)
6C20 FORMAT(8H0DEBUG 3-, (6E20.8))
2000 DO 2500 K=1,KT
    IF(S(K,J)) 2200, 2500, 2100
2100 X=DE(K)-W(K,J)-1.0E-5
    Y=DE(K)+W(K,J)+1.0E-5
    DO 2150 L=1,LT
        IF(X-EPS(L)) 2130, 2130, 2150
2130 IF(Y-EPS(L)) 2500, 2140, 2140
2140 XABS(L)=XABS(L)+1.5708*S(K,J)
2150 CONTINUE
    GO TO 2500
2200 X=W(K,J)**2
    Y=ABSF(S(K,J))**X
    DO 2250 L=1,LT
        XARS(L)=XABS(L)+Y/(X+(FPS(L)-DE(K))**2)
2250 CONTINUE
    IF1LCD) 3000, 2900, 2900
2900 IF(OMEGA(N)-EMIN) 3000, 2910, 2910
2910 WRITE OUTPUT TAPE 6, 6030, (XABS(L),L=1,LT)
6030 FORMAT(8H0DEBUG 4--,(6E20.8))
3000 LTP=LT-1
    X=0.0
    DO 3100 L=1,LTP
3100 X=X+0.5*(EPS(L+1)-EPS(L))*(1.0/XABS(L+1)+1.0/XABS(L))
    ABS(N,J)=X/DCMEGA
3500 CONTINUE
4000 DO 4100 K=1,KT
    IF(DE(K)-OMEGA(N)) 4100,4200, 4200
4100 CONTINUE
    KT=0

```

```

GO TO 500
4200 KP=1
4210 DE(KP)=DE(K)
DO 4250 J=1,6
S(KP,J)=S(K,J)
4250 W(KP,J)=W(K,J)
K=K+1
IF(K-KT) 4260,4260, 4280
4260 KP=KP+1
GO TO 4210
4280 KT=KP
500 CONTINUE
LC=100
DO 600 N=1,NOM
E=8065.73*OMEGA(N)
WAVE=12398.1/OMEGA(N)
IF(LC-50) 550, 550, 525
525 WRITE OUTPUT TAPE 6, 5010,K1,IBETA,OMEGA,DOMEGA, OMEGA(NOMEGA)
      WRITE OUTPUT TAPE 6, 5020
LC=3
550 WRITE OUTPUT TAPE 6, 5030, OMEGA(N),E,WAVE, (ABS(N,J),J=1,6)
LC=LC+1
600 CONTINUE
RETURN
5000 FORMAT(22HOKT GREATER THAN KDIM-,E20.8,2110)
5010 FORMAT(16H1MEAN FREE PATH-10X,3H1E-,12.5X,5HBEITA=,12.5X,7HENERGY=,XMF
11PE9.3,1H(.1PE9.3,1H),1PE9.3)
5020 FORMAT(1H0.5X,6HENERGY,8X,6HENERGY,5X,11HWAVE LENGTH,26X,18HMEAN F
1RE E PATH(CM)/1H ,6X,4H(EV),9X,6H(1/CM),6X,1CH(ANGSTROM),5X,8HALPHAXMF
2(1),6X,8HALPHA(2),6X,8HALPHA(3),6X,8HALPHA(4),6X,8HALPHA(5),6X,8HALPH
3LPHA(6)/
5030 FORMAT(1P9E14.4)
5035 FORMAT(21H ENERGY TABLE FILLED-,3I10,3E20.8)
5040 FORMAT(21H1INCORRECT LINE TAPE-,10X,11HELEMENT ID=,I3,16HTAPE ELEM
1ENT ID=,I3)
5045 FORMAT(21H1INCORRECT LINE TAPE-,10X,15HTE'PERATURE ID=,I3,20HTAPE XMF
F7

```

1 TEMPERATURE ID=131
END

XMF P F7
XMF P

```

*          FORTRAN
*          SUBROUTINE RMEAN
C          TO ACCUMULATE AND PRINT PARTIAL ROSSELAND MEAN OPACITIES-
COMMON NENGY, OMEGA, NOMEA, DOMEA, A35, RHOI, RHOE,
1 LDIM, KDIM, WC, IBETA, TEMP, K1
DIMENSION OMEGA(2000), ABS(2000,6), RHOI(6), RHOE(6), WC(6),
1 XABS(2000)
NUMP=NOMEGA-1
DO 100 N=1,NUMP
X=(OMEGA(N)+OMEGA(N+1))*0.5/TEMP
Y=EXP(-X)
XABS(N)=0.0385*X**4/TEMP*Y/(1.0-Y)**3
100 CONTINUE
DO 120 J=1,6
120 WC(J)=0.0
LC=100
DO 500 N=3,NUMP,2
DO 150 J=1,6
150 WC(J)=WC(J)+DOMEA(N-1)*ABS(N-2)*ABS(N-2,J)
1 +4.0*XABS(N-1)*ABS(N-1,J)+XABS(N)*ABS(N,J)
E=8065.73*OMEGA(N+1)
WAVE=12398.1/OMEGA(N+1)
IF(LC-50) 300, 300, 200
300 WRITE OUTPUT TAPE 6, 1000,1,1,IBETA,OMEGA0,DOMEA,OMEGA(N+1)
WRITE OUTPUT TAPE 6, 1010
LC=3
300 WRITE OUTPUT TAPE 6, 1020, OMEGA(N+1),E,WAVE, WC
LC=LC+1
500 CONTINUE
500 RETURN
1000 FORMAT(24H1ROSSELAND MEAN OPACITY-,10X,3HID=,12,5X,5HBETA=,12,5X,7RMEAN F1
1HENERGY=,1PE9.3,1H(,1PE9.3,1H),1PE9.3)
1010 FORMAT(1H0,5X,6HENERGY,5X,11HWAVE LENGTH,26X,16HMEAN ORMEAN F2
1PACITY(CM)/1H,6X,4H(1/CM),9X,6H(1/CM),6X,10H(ANGSTROM),5X,8HALPHA(1RMELAN F2
2),6X,8HALPHA(2),6X,8HALPHA(3),6X,8HALPHA(4),6X,8HALPHA(5),6X,8HALPHA(6),/3HA(6)/
1020 FORMAT(1P9E14.4)
END

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